10/530,858A Yong Chu 10-09-2007

$%^STN;HighlightOn=;HighlightOff=;

Connecting via Winsock to STN

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LOGINID:ssptaylc1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 02	LMEDLINE coverage updated
NEWS	3	JUL 02	SCISEARCH enhanced with complete author names
NEWS	4	JUL 02	CHEMCATS accession numbers revised
NEWS	5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS	6	JUL 16	CAplus enhanced with French and German abstracts
NEWS	7	JUL 18	CA/CAplus patent coverage enhanced
NEWS	8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	9	JUL 30	USGENE now available on STN
NEWS	10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	11	AUG 06	BEILSTEIN updated with new compounds
NEWS	12	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	13	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS	14	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS	15	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	16	AUG 27	USPATOLD now available on STN
NEWS	17	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	18	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	19	SEP 13	FORIS renamed to SOFIS
NEWS	20	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	21	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS	22	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS	23	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	24	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 09:58:05 ON 09 OCT 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:58:19 ON 09 OCT 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 OCT 2007 HIGHEST RN 949630-10-8
DICTIONARY FILE UPDATES: 8 OCT 2007 HIGHEST RN 949630-10-8

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
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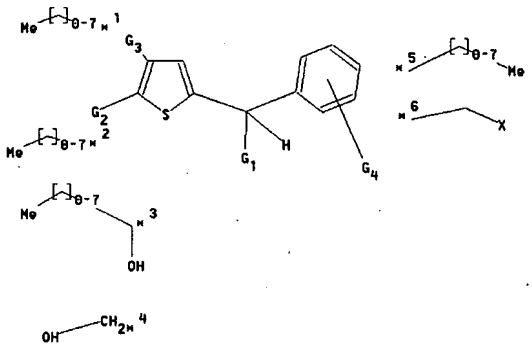

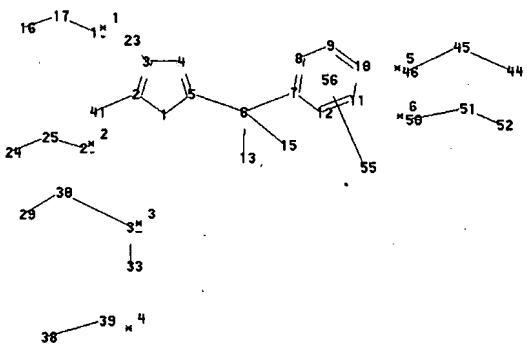

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6 13 15 16 17 18 23 24 25 26 29 30 32 33 38 39 41 44 45 46 50 51 52 55
ring nodes :
1 2 3 4 5 7 8 9 10 11 12
chain bonds :
2-41 3-23 5-6 6-7 6-13 6-15 16-17 17-18 24-25 25-26 29-30 30-32 32-33 38-39 44-45 45-46 50-51 51-52
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-5 2-3 2-41 3-4 3-23 4-5 6-13 32-33
exact bonds :
5-6 6-7 6-15 16-17 17-18 24-25 25-26 29-30 30-32 38-39 44-45 45-46 50-51
51-52
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

G1:H,OH

G2:H,CH3,[*1],[*2],[*3],[*4]

G3:H,CH3,[*1]

G4:H,CH3,X,[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 23:CLASS 24:CLASS 25:CLASS
26:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 38:CLASS 39:CLASS 41:CLASS 44:CLASS 45:CLASS
46:CLASS 50:CLASS 51:CLASS 52:CLASS 55:CLASS 56:Atom

L1 STRUCTURE UPLOADED

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=> d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 09:58:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     5312 TO ITERATE

 37.7% PROCESSED     2000 ITERATIONS                                  50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       101870 TO   110610
PROJECTED ANSWERS:            3709 TO     5533

L2           50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:59:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   105841 TO ITERATE

100.0% PROCESSED   105841 ITERATIONS                            4491 ANSWERS
SEARCH TIME: 00.00.01

L3          4491 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     172.55     172.76

FILE 'CAPLUS' ENTERED AT 09:59:14 ON 09 OCT 2007
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FILE COVERS 1907 - 9 Oct 2007  VOL 147 ISS 16
FILE LAST UPDATED: 8 Oct 2007  (20071008/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:
```

http://www.cas.org/infopolicy.html

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=> s l3
L4          1044 L3

=> s l3 and thiophene
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           42509 THIOPHENE
            6581 THIOPHENES
           44368 THIOPHENE
                 (THIOPHENE OR THIOPHENES)
L5           380 L3 AND THIOPHENE

=> s l5 and benzoate
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            6704 BENZOATES
           72477 BENZOATE
                 (BENZOATE OR BENZOATES)
L6            23 L5 AND BENZOATE

=> s l6 and synthesis
         1343702 SYNTHESIS
               3 SYNTHESISES
           70686 SYNTHESES
         1383212 SYNTHESIS
                 (SYNTHESIS OR SYNTHESISES OR SYNTHESES)
L7             1 L6 AND SYNTHESIS

=> s l6 and prepare
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            1555 PREPARES
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                 (PREPARE OR PREPARES)
          133013 PREP
            2320 PREPS
          135118 PREP
                 (PREP OR PREPS)
          145664 PREPARE
                 (PREPARE OR PREP)
L8             0 L6 AND PREPARE

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          330246 REDUCTION
            5677 REDUCTIONS
          333074 REDUCTION
                 (REDUCTION OR REDUCTIONS)
          955587 REDN
           53830 REDNS
          989528 REDN
                 (REDN OR REDNS)
         1138938 REDUCTION
                 (REDUCTION OR REDN)
L9             0 L6 AND REDUCTION

=> d l6 ibib abs hitstr tot

L6   ANSWER 1 OF 23  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:472885  CAPLUS  Full-text
DOCUMENT NUMBER:          147:95348
TITLE:                    The palladium-catalyzed addition of aryl- and
```

heteroarylboronic acids to aldehydes

AUTHOR(S): Qin, Changming; Wu, Huayue; Cheng, Jiang; Chen, Xi'an; Liu, Miaochang; Zhang, Weiwei; Su, Weike; Ding, Jinchang

CORPORATE SOURCE: College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, 325027, Peop. Rep. China

SOURCE: Journal of Organic Chemistry (2007), 72(11), 4102-4107
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

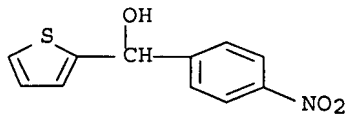
LANGUAGE: English

AB Reaction of aryl- or heteroarylboronic acids with aldehydes, in the presence of PdCl2 and P(1-Nap)3, afforded carbinol derivs. in good to excellent yields. The efficiency of this reaction was demonstrated by the compatibility with nitro, cyano, acetamido, acetoxy, acetyl, carboxyl, trifluoromethyl, fluoro, and chloro groups and the possibility of involving aliph. aldehyde or hindered substrates. Moreover, the rigorous exclusion of air/moisture is not required in these transformations.

IT 40310-37-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aryl and heteroaryl substituted alcs. via palladium-phosphine-catalyzed addn. of aryl- or heteroarylboronic acids with aldehydes)

RN 40310-37-0 CAPLUS

CN 2-Thiophenemethanol, .alpha.-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:358531 CAPLUS Full-text

DOCUMENT NUMBER: 143:59757

TITLE: Deprotonation of thiophenes using lithium magnesates

AUTHOR(S): Bayh, Omar; Awad, Hacan; Mongin, Florence; Hoarau, Christophe; Trecourt, Francois; Queguiner, Guy; Marsais, Francis; Blanco, Fernando; Abarca, Belen; Ballesteros, Rafael

CORPORATE SOURCE: Laboratoire de Chimie Organique Fine et Heterocyclique, UMR 6014, IRCOF, CNRS, Universite et INSA de Rouen, Mont-Saint-Aignan, 76131, Fr.

SOURCE: Tetrahedron (2005), 61(20), 4779-4784
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

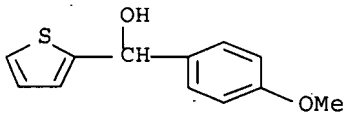
OTHER SOURCE(S): CASREACT 143:59757

AB Thiophene was regioselectively deprotonated at C-2 on treatment with 1/3 equiv of Bu3MgLi in THF at room temp. The lithium arylmagnesate formed was either trapped with electrophiles or cross-coupled in a one-pot procedure with aryl halides under palladium catalysis. 2-Chlorothiophene and 2-methoxythiophene

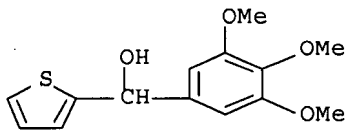
were similarly deprotonated at C-5 under the same reaction conditions. The enhancement of the reactivity of the base using TMEDA was evidenced using 1H NMR spectroscopy.

IT 40310-33-6P 356552-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(deprotonation of thiophenes using lithium magnesates and substitution or coupling reactions)

RN 40310-33-6 CAPLUS
CN 2-Thiophenemethanol, .alpha.-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 356552-33-5 CAPLUS
CN 2-Thiophenemethanol, .alpha.-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:275943 CAPLUS Full-text
DOCUMENT NUMBER: 136:310050
TITLE: Preparation of new retinoids for the treatment of emphysema, cancer and dermatological disorders
INVENTOR(S): Lapierre, Jean-Marc; Rotstein, David Mark; Sjogren, Eric Brian
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 161 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028810	A2	20020411	WO 2001-EP11017	20010924
WO 2002028810	A3	20020926		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,

UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2422805	A1	20020411	CA 2001-2422805		20010924
AU 200189913	A	20020415	AU 2001-89913		20010924
AU 2001289913	A2	20020415	AU 2001-289913		20010924
BR 2001014344	A	20030701	BR 2001-14344		20010924
EP 1324970	A2	20030709	EP 2001-969762		20010924
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HU 200303006	A2	20031229	HU 2003-3006		20010924
JP 2004510728	T	20040408	JP 2002-532198		20010924
NZ 524603	A	20041029	NZ 2001-524603		20010924
RU 2282616	C2	20060827	RU 2003-112608		20010924
US 2002082265	A1	20020627	US 2001-968425		20011001
US 6777418	B2	20040817			
ZA 2003001978	A	20040625	ZA 2003-1978		20030311
NO 2003001480	A	20030520	NO 2003-1480		20030401
MX 2003PA02861	A	20030714	MX 2003-PA2861		20030401
IN 2003CN00453	A	20050415	IN 2003-CN453		20030401
HK 1061229	A1	20070831	HK 2004-104315		20040615
PRIORITY APPLN. INFO.:			US 2000-237459P	P	20001002
			WO 2001-EP11017	W	20010924

OTHER SOURCE(S): MARPAT 136:310050
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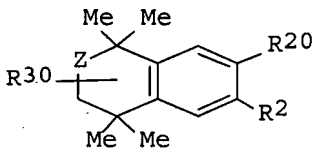

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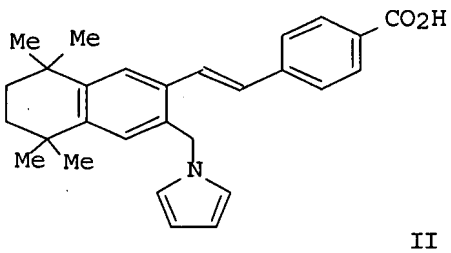


II

AB The current invention provides novel retinoid compds., e.g., I [Z = (CH2)n; R20 = AcBdXR1; R30 = (R3)t; n = 0 - 2; c = 0, 1; d = 0, 1; A = C(:O), C(:CH2), C(:NR4), CR5R6; B = C(:O)O, OC(:O), C(:O)NH, NHC(:O), NHC(:O)NH, CR7:CR8, CR7:CR8C(:O), C.tplbond.C, C.tplbond.CC(:O), CH2O, CH2S, OCH2, SCH2,COCH2, CH2CO; X = aryl, heteroaryl; R1 = C(:O)R9; R2 = (CR10R11)mYpR12, heteroaryl, ZL, CR14:CR15; R3 = H, alkyl, OH, oxo; t = 1,2 for n = 1, 2 and t = 1 for n = 0; R4 = H, alkyl, OH, alkoxy, NH2; R5, R6 = H, alkyl; CR5R6 = cycloalkyl; R7, R8 = H, alkyl; R9 = alkyl, cycloalkyl, cycloalkylalkyl, OH, alkoxy, aryloxy, cycloalkoxy, (cycloalkyl)alkoxy, arylalkoxy, NH2, (di)alkylamino, heteroalkoxy, heteroalkylamino, heteroalkylthio, heterocyclyl, heterocyclylalkyl; m = 1 - 10, p = 0, 1; R10, R11 = H, alkyl, OH,

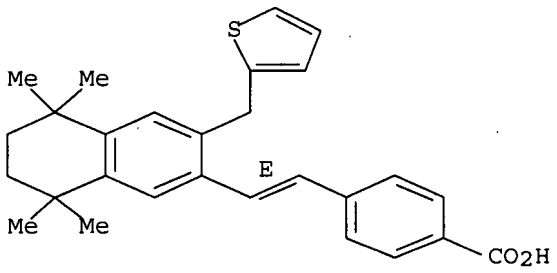
hydroxyalkyl; Y = O, S(O)q, NR13; q = 0 - 2; R12 = H, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl, arylalkyl, heteroaryl, heteroarylalkyl, acyl, alkoxycarbonyl, carbamoyl, heteroalkyl, etc.; R13 = H, alkyl; R14, R15, R16 = H, alkyl; L = heteroaryl, heteroarylalkyl, heteroalkyl; R17 = alkyl; R18, R19 = H, alkyl] or a pharmaceutically acceptable salt, solvate or hydrate thereof, methods for their synthesis, use of I for the prepn. of medicaments for treating or preventing emphysema, cancer and dermatol. disorders and pharmaceutical compns. suitable for these disorders. Thus, retinoid II was prepd. from 2-bromo-3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalene via metalation-formylation with BuLi in hexane then N-formylpiperidine, Horner-Emmons reaction with 4-[(MeO)2P(O)CH2]C6H4CO2Me in PhMe contg. potassium tert-pentylate, benzylic bromination with NBS in CCl4 contg. catalytic (PhCO2)2O, amination with pyrrole in N-methylpyrrolidine an sapon. with NaOH in EtOH. The above were tested for their retinoid receptor binding ability [for II: IC50 = 260 nM vs. .alpha., IC50 = 140 nM vs. .beta., IC50 = 170 nM vs. .gamma.].

IT 410528-40-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of new retinoids for the treatment of emphysema, cancer and dermatol. disorders)

RN 410528-40-4 CAPLUS

CN Benzoic acid, 4-[(1E)-2-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(2-thienylmethyl)-2-naphthalenyl]ethenyl]- (9CI) (CA INDEX NAME)

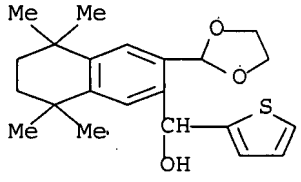
Double bond geometry as shown.



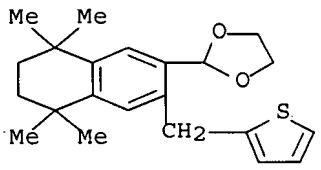
IT 410528-80-2P 410528-82-4P 410529-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of new retinoids for the treatment of emphysema, cancer and dermatol. disorders)

RN 410528-80-2 CAPLUS

CN 2-Thiophenemethanol, .alpha.-[3-(1,3-dioxolan-2-yl)-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl]- (9CI) (CA INDEX NAME)

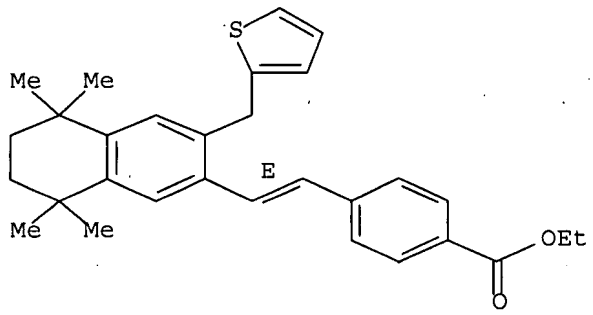


RN 410528-82-4 CAPLUS
CN 1,3-Dioxolane, 2-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(2-thienylmethyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)



RN 410529-91-8 CAPLUS
CN Benzoic acid, 4-[(1E)-2-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(2-thienylmethyl)-2-naphthalenyl]ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

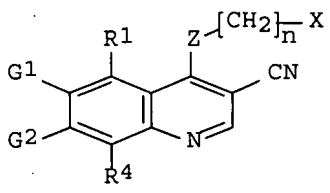


L6 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:672213 CAPLUS Full-text
DOCUMENT NUMBER: 135:226901
TITLE: Preparation of 3-cyanoquinolines as protein tyrosine kinase inhibitors
INVENTOR(S): Wissner, Allan; Tsou, Hwei-ru; Berger, Dan M.; Floyd, Middleton B., Jr.; Hamann, Philip R.; Zhang, Nan; Salvati, Mark E.; Frost, Philip
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 68 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

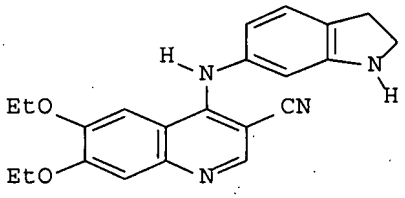
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6288082	B1	20010911	US 1999-406573		19990924
PRIORITY APPLN. INFO.:			US 1998-150693P	P	19980929

OTHER SOURCE(S): MARPAT 135:226901

GI



I



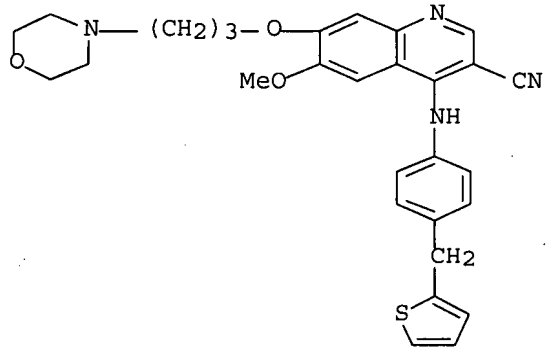
II

AB The title compds. [I; X = (un)substituted bicyclic aryl or bicyclic heteroaryl ring system of 8-12 atoms where the bicyclic heteroaryl ring contains 1-4 heteroatoms selected from N, O and S; Z = (un)substituted NH, O, S; G1, G2, R1, R4 = H, halo, alkyl, etc.; n = 0-1], useful as antineoplastic agents and in the treatment of polycystic kidney disease, were prepd. Thus, Me 2-amino-4,5-diethoxybenzoate was N-condensed with HCNMe2/POCl3 and the product cyclocondensed with MeCN to give, after POCl3 treatment, 4-chloro-6,7-diethoxyquinoline-3-carbonitrile which was aminated by 6-aminoindoline to give title compd II. Data for biol. activity (inhibition of EGFR kinase, KDR, Eck, Mek-Erk) of I were given.

IT 263170-95-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-cyanoquinolines as protein tyrosine kinase inhibitors)

RN 263170-95-2 CAPLUS

CN 3-Quinolinecarbonitrile, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[4-(2-thienylmethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:294962 CAPLUS Full-text

DOCUMENT NUMBER: 134:311098

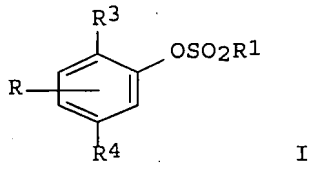
TITLE: Preparation of [[(benzofuranylbiphenylyl)oxy]sulfonyl] benzoates and analogs as PTPase inhibitors

INVENTOR(S): Malamas, Michael S.; Adebayo, Folake O.; Dollings, Paul J.

PATENT ASSIGNEE(S): American Home Products Corporation, USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6221902	B1	20010424	US 1999-307888		19990510
US 6310081	B1	20011030	US 2001-797019		20010301
PRIORITY APPLN. INFO.:			US 1998-99365P	P	19980512
			US 1999-307888	A3	19990510

OTHER SOURCE(S): MARPAT 134:311098
GI

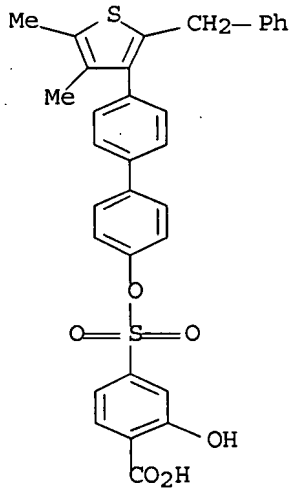


I

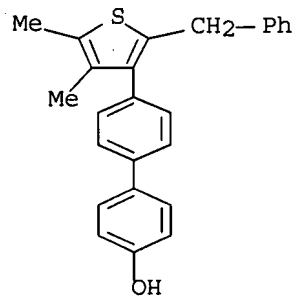
AB Title compds. [I; R = 4-heteroarylphenyl; R1 = e.g., ZCO2R5; R3,R4 = H, halo, alkyl, alkoxy, etc.; R5 = H, alkyl, aryl, etc.; Z = (OR5- or O2CR5-substituted) phenylene] were prepd. Thus, 4-BrC6H4COCH2Br was etherified by PhOH and the product cyclized to give 3-(4- bromophenyl)benzofuran which was condensed with 4-(MeO)C6H4B(OH)2 and the product converted in 4 steps to I [R = 4-[4-(PhCH2Z1)C6H4], R1 = C6H3(OH)(CO2H)-3,4, R3 = R4 = H, Z1 = benzofuran-2,3-diyl]. Data for biol. activity of I were given.

IT 250279-02-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of [[(benzofuranylbiphenylyl)oxy]sulfonyl]benzoates and analogs as PTPase inhibitors)

RN 250279-02-8 CAPLUS
CN Benzoic acid, 4-[[[4'-[4,5-dimethyl-2-(phenylmethyl)-3-thienyl][1,1'-biphenyl]-4-yl]oxy]sulfonyl]-2-hydroxy- (CA INDEX NAME)



IT 250279-23-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of [[(benzofuranylbiphenylyl)oxy]sulfonyl]benzoates and analogs as PTPase inhibitors)
RN 250279-23-3 CAPLUS
CN [1,1'-Biphenyl]-4-ol, 4'-[4,5-dimethyl-2-(phenylmethyl)-3-thienyl]- (9CI) (CA INDEX NAME)



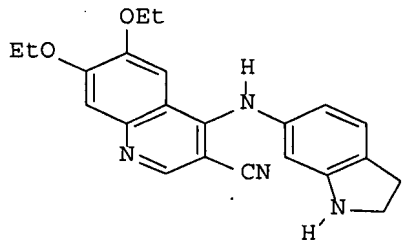
REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:227652 CAPLUS Full-text
DOCUMENT NUMBER: 132:265101
TITLE: Preparation of 3-cyanoquinolines as protein tyrosine kinase inhibitors
INVENTOR(S): Wissner, Allan; Tsou, Hwei-Ru; Berger, Dan Maarten; Floyd, Middleton Brawner, Jr.; Hamann, Philip Ross; Zhang, Nan; Salvati, Mark Ernest; Frost, Philip
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: PCT Int. Appl., 195 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000018761	A1	20000406	WO 1999-US22054		19990922
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2344169	A1	20000406	CA 1999-2344169		19990922
AU 9961593	A	20000417	AU 1999-61593		19990922
AU 763669	B2	20030731			
EP 1117659	A1	20010725	EP 1999-948410		19990922
EP 1117659	B1	20031203			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
HU 200103520	A2	20020228	HU 2001-3520		19990922
JP 2002525369	T	20020813	JP 2000-572221		19990922
NZ 510551	A	20030328	NZ 1999-510551		19990922
AT 255575	T	20031215	AT 1999-948410		19990922
PT 1117659	T	20040430	PT 1999-948410		19990922
ES 2211175	T3	20040701	ES 1999-948410		19990922
SK 284846	B6	20051201	SK 2001-413		19990922
TW 233437	B	20050601	TW 1999-88116630		19990929
NO 2001001575	A	20010528	NO 2001-1575		20010328
MX 2001PA03230	A	20011011	MX 2001-PA3230		20010328
IN 2001KN00370	A	20060303	IN 2001-KN370		20010329
ZA 2001002729	A	20020703	ZA 2001-2729		20010403
HK 1035188	A1	20040402	HK 2001-105823		20010817
PRIORITY APPLN. INFO.:			US 1998-162802	A	19980929
			WO 1999-US22054	W	19990922

OTHER SOURCE(S): MARPAT 132:265101
GI



II

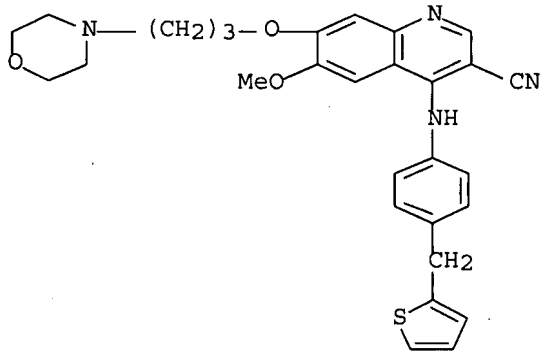
AB X(CH2)nZZ1CN [I; X = (un)substituted bicyclic (hetero)aryl or LTA; A = (un)substituted phenylene, -pyridinediyl, -pyrimidinediyl; T = O, S, (alkyl)imino(alkylene), oxyalkylene, etc.; Z = O, S, (alkyl or alkanoyl)imino; Z1 = 2-unsubstituted-5,6,7,8-(un)substituted quinoline-4,3-diyl; n = 0 or 1] were prepd. Thus, Me 2-amino-4,5- diethoxybenzoate was N-condensed with

HCNMe2/POCl3 and the product cyclocondensed with MeCN to give, after POCl3 treatment, 4-chloro-6,7-diethoxyquinoline-3-carbonitrile which was aminated by 6-aminoindoline to give title compd II. Data for biol. activity of I were given.

IT 263170-95-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-cyanoquinolines as protein tyrosine kinase inhibitors)

RN 263170-95-2 CAPLUS

CN 3-Quinolinecarbonitrile, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[4-(2-thienylmethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



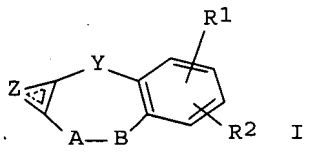
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:104514 CAPLUS Full-text
DOCUMENT NUMBER: 130:153583
TITLE: Tricyclic benzazepine oxytocin and vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Sum, Fuk-Wah
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 110 pp., Cont.-in-part of U.S. Ser. No. 254,823.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5869483	A	19990209	US 1996-639014	19960424
US 5512563	A	19960430	US 1994-254823	19940613
NZ 299340	A	20000825	NZ 1994-299340	19940728
US 5693635	A	19971202	US 1996-662546	19960613
US 5834461	A	19981110	US 1997-874314	19970613
US 5843952	A	19981201	US 1997-889858	19970708
PRIORITY APPLN. INFO.:			US 1993-100003	B2 19930729
			US 1994-254823	A2 19940613
			NZ 1994-264116	A1 19940728
			US 1996-639014	A2 19960424
			US 1996-663400	B1 19960613

OTHER SOURCE(S): MARPAT 130:153583
GI



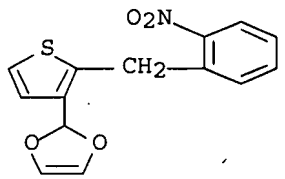
I

AB This invention relates to title compds. I wherein: Y = e.g., (CH2)n, O, S wherein n is an integer from 0-2; A-B is (CH2)mNR3 or NR3(CH2)m , wherein m is an integer from 1-2, provided that when Y is (CH2)n and n=2, m may also be zero and when n is zero, m may also be three, provided also that when Y is (CH2)n and n is 2, m may not also be two; R1 = e.g., H, halo, OH; R2 = e.g., H, halo, OH; R3 is the moiety COAr where Ar is selected from, e.g., substituted Ph, (un)substituted 5-indolyl; the arom. Z ring represents, e.g., fused (un)substituted Ph, 5- or 6-membered atom. heterocycle, that exhibit antagonist activity at V1 and/or V2 receptors and exhibit in vivo vasopressin antagonist activity, methods for using such compds. in treating diseases characterized by excess renal reabsorption of water, and processes for prepg. such compds. I are also antagonists of the peptide hormone oxytocin and are useful in the control of premature birth. Thus, e.g., acylation of 6,11-dihydro-5H- dibenz[b,e]azepine (prepn. given) with 4-[(2-methylbenzoyl)amino]benzoyl chloride (prepn. given) afforded N-[4-[(6,11-dihydro-5H-dibenz[b,e]azepin- 5-yl)carbonyl]phenyl]-2-methylbenzamide which exhibited binding to rat hepatic V1 receptors and rat kidney medullary V2 receptors with IC50 = 0.15 and 0.068 .mu.M, resp., and oxytocin receptor binding with IC50 = 2.9 .mu.M.

IT 178448-00-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tricyclic benzazepine oxytocin and vasopressin antagonists)

RN 178448-00-5 CAPLUS

CN 1,3-Dioxole, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX NAME)



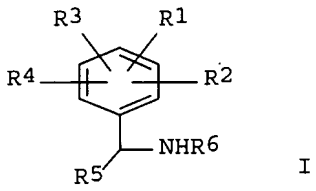
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:7963 CAPLUS Full-text

DOCUMENT NUMBER: 130:52423
TITLE: Preparation of benzylamine derivatives having excellent ileal bile acid transporter inhibitory activity
INVENTOR(S): Ishihara, Sadao; Saito, Fujio; Masuko, Hidekazu; Kono, Keita
PATENT ASSIGNEE(S): Sankyo Company, Ltd., Japan
SOURCE: PCT Int. Appl., 305 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9856757	A1	19981217	WO 1998-JP2531	19980609
W: AU, BR, CA, CN, CZ, HU, ID, IL, KR, MX, NO, NZ, PL, RU, TR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9875521	A	19981230	AU 1998-75521	19980609
JP 11060548	A	19990302	JP 1998-161819	19980610
PRIORITY APPLN. INFO.:			JP 1997-153837 A	19970611
			WO 1998-JP2531 W	19980609

OTHER SOURCE(S): MARPAT 130:52423
GI



I

AB Benzylamine derivs. represented by general formula (I) or pharmacol. acceptable salts thereof [wherein R1 represents substituted C6-10 aryl, optionally substituted tetrazolyl, (C3-6 cycloalkyl)carbamoyl, (C1-6 alkyl)sulfonylcarbamoyl, SO3H, C1-6 alkylsulfonyl, C1-6 alkylsulfinyl, optionally substituted (C6-10 aryl)sulfonylcarbamoylamino, etc.; R2, R3, and R4 each represents hydrogen, C1-6 alkyl or alkoxy, OH, halo, NH2, mono(C1-6 alkyl)amino, di(C1-6 alkyl)amino; R5 represents optionally substituted C6-10 aryl, optionally substituted and/or optionally benzene-fused thienyl, pyrrolyl, 1,1-dioxothienyl, thiazolyl, or oxazolyl; and R6 represents C1-10 alkyl, a group having -W-R7, or optionally substituted C7-16 aralkyl; wherein W represents a single bond or C1-6 alkylene and R7 = optionally substituted and/or benzene-fused C3-6 cycloalkyl; provided when R1 is C1-6 alkylsulfonyl or C1-6 alkylsulfinyl, then R6 is not C1-10 alkyl] are prepd. Also claimed is a pharmaceutical compn. contg. I for inhibiting ileum-type bile acid transporter. Thus, NaN3 and tri(n-butyl)tin chloride were added to a soln. of N-(1-ethylpentyl)[phenyl(3-cyanophenyl)methyl]amine in toluene and the resulting mixt. was stirred at room temp. for 30 min and refluxed fro 2 h to give N-(1-ethylpentyl)[phenyl[3-(1H-tetrazol-5-yl)phenyl]methyl]amine (II) which at 10 .mu.g/mL in vitro inhibited by 72% the uptake of radio labeled taurocholic acid to rat everted ileal rings. Two isomers of N-[4-[phenyl-[[N-

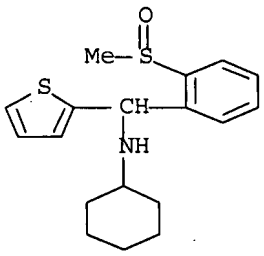
(1R)-phenylethyl]amino]methyl]phenyl]-N'-p- toluenesulfonylurea in vitro showed IC50 of 1.2 and 0.8 .mu.g/mL for inhibiting the uptake of radio labeled taurocholic acid in Caco-2 cells expressing ileal bile acid transporter. A tablet formulation contg. II was prepd.

IT 217496-85-0P 217497-78-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzylamine derivs. as inhibitors of ileal bile acid transporter)

RN 217496-85-0 CAPLUS
CN 2-Thiophenemethanamine, N-cyclohexyl-.alpha.-[2-(methylsulfinyl)phenyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

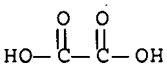
CM 1

CRN 217496-84-9
CMF C18 H23 N O S2



CM 2

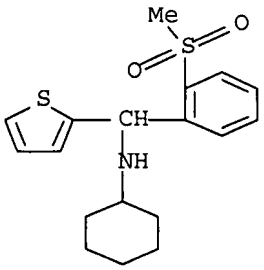
CRN 144-62-7
CMF C2 H2 O4



RN 217497-78-4 CAPLUS
CN 2-Thiophenemethanamine, N-cyclohexyl-.alpha.-[2-(methylsulfonyl)phenyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

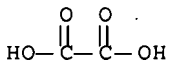
CM 1

CRN 217497-77-3
CMF C18 H23 N O2 S2

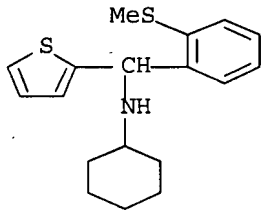


CM 2

CRN 144-62-7
CMF C2 H2 O4



IT 217497-92-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of benzylamine derivs. as inhibitors of ileal bile acid transporter)
RN 217497-92-2 CAPLUS
CN 2-Thiophenemethanamine, N-cyclohexyl-.alpha.-[2-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

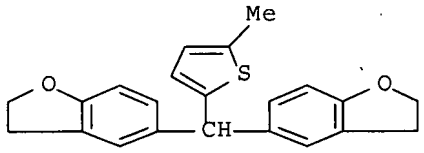
L6 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:776987 CAPLUS Full-text
DOCUMENT NUMBER: 130:109867
TITLE: Kinetics of the Friedel-Crafts Alkylations of Heterocyclic Arenes: Comparison of the Nucleophilic Reactivities of Aromatic and Nonaromatic .pi.-Systems
AUTHOR(S): Gotta, Matthias F.; Mayr, Herbert
CORPORATE SOURCE: Institut fuer Organische Chemie der Ludwig-Maximilians-Universitaet Muenchen, Munich,

80333, Germany
SOURCE: Journal of Organic Chemistry (1998), 63(26), 9769-9775
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

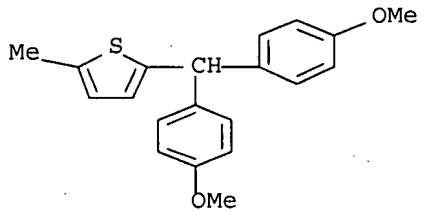
AB The kinetics of the reactions of benzhydryl cations with heteroarenes (N-methylpyrrole, furan, 2-methylfuran, and 2-methylthiophene) have been detd. photometrically in dichloromethane, and the reaction products have been completely characterized by 1H and 13C NMR spectroscopy. The reactions follow second-order kinetics with rate-limiting formation of the .sigma.-adducts. The second-order rate consts. correlate linearly with the electrophilicity parameter E of the benzhydryl cations. This allows the detn. of the reactivity parameters N and s for the heteroarenes according to the linear free enthalpy relationship log k = s(E + N) (Mayr, H.; Patz, M. Angew. Chem., Int. Ed. Engl. 1994, 33, 938-957). The nucleophilicity parameters N thus defined allow a direct comparison of the nucleophilic reactivities of arom. and nonarom. .pi.-systems. Since N correlates linearly with .sigma.+arene, it becomes possible to derive N parameters for arenes and heteroarenes with known .sigma.+ parameters and to calc. abs. rate consts. for their reactions with carbenium ions and diazonium ions. Applications of the reactivity parameters thus detd. for the quant. and qual. prediction of the rates of electrophilic arom. substitutions are discussed.

IT 219723-35-0P 219723-36-1P 219751-12-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Lewis acid catalyzed reactions of diarylmethyl derivs. with heteroarenes in CH2Cl2)

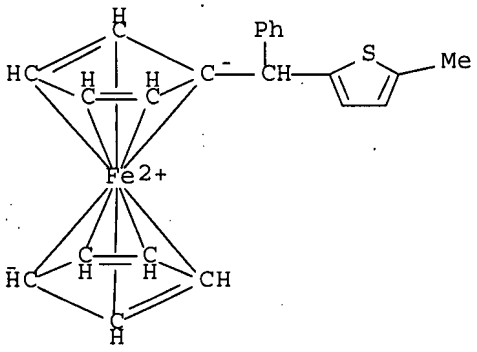
RN 219723-35-0 CAPLUS
CN Benzofuran, 5,5'-[(5-methyl-2-thienyl)methylene]bis[2,3-dihydro- (9CI) (CA INDEX NAME)



RN 219723-36-1 CAPLUS
CN Thiophene, 2-[bis(4-methoxyphenyl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 219751-12-9 CAPLUS
CN Ferrocene, [(5-methyl-2-thienyl)phenylmethyl]- (9CI) (CA INDEX NAME)

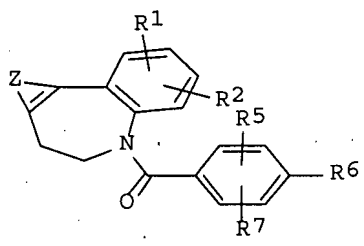


REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:366893 CAPLUS Full-text
DOCUMENT NUMBER: 129:54301
TITLE: Preparation of tricyclic benzazepine vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Reich, Marvin Fred
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 103 pp., Cont.-in-part of U. S. 5,512,563.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5760031	A	19980602	US 1996-637911	19960425
US 5512563	A	19960430	US 1994-254823	19940613
NZ 299340	A	20000825	NZ 1994-299340	19940728
PRIORITY APPLN. INFO.:			US 1993-100003 B2	19930729
			US 1994-254823 A2	19940613
			NZ 1994-264116 A1	19940728

OTHER SOURCE(S): MARPAT 129:54301
GI



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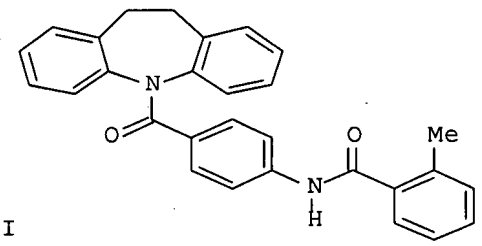


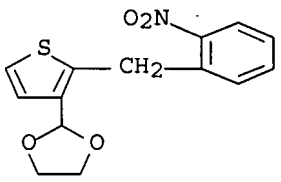
II

AB The title compds. [I; R1 = H, Cl, F, etc.; R2 = H, Cl, Br, etc.; R1R2 = methylenedioxy, ethylenedioxy; R5 = H, Me, Et, etc.; R6 = N(Ra)COAr', CON(Ra)Ar', etc. (Ra = H, Me, Et; Ar' = (un)substituted Ph, thienyl, etc.); R7 = H, Me, Et, etc.; Z = (un)substituted fused oxazole, Ph], which exhibit antagonist activity at V1 and/or V2 receptors and in vivo vasopressin antagonist activity as well as antagonist activity at oxytocin receptors, and as such useful in treating diseases characterized by excess renal reabsorption of water (e.g., congestive heart failure, nephrotic syndrome, hyponatremia, coronary vasospasm, cardiac ischemia, renal vasospasm, liver cirrhosis, brain edema, cerebral ischemia, cerebral hemorrhage-stroke), were prepd. Thus, reaction of 4-[(2- methylbenzoyl)amino]benzoyl chloride with 10,11-dihydro-5H-dibenz[b,f]azepine in the presence of 4-(dimethylamino)pyridine in pyridine at 80.degree. for 18 h followed by the addn. of NaH afforded the compd. II which showed IC50 of 2.5 .mu.M against rat hepatic V1 receptor binding and IC50 of 0.86 .mu.M against rat kidney medullary V2 receptor binding.

IT 167770-26-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of tricyclic benzazepine vasopressin antagonists)

RN 167770-26-5 CAPLUS

CN 1,3-Dioxolane, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:289524 CAPLUS Full-text
DOCUMENT NUMBER: 128:321569
TITLE: Preparation of tricyclic benzazepine vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Reich, Marvin Fred
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 101 pp., Cont.-in-part of U.S. Ser. No. 5,512,563.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5747487	A	19980505	US 1996-638067	19960425
US 5512563	A	19960430	US 1994-254823	19940613
NZ 299340	A	20000825	NZ 1994-299340	19940728
PRIORITY APPLN. INFO.:			US 1993-100003 B2	19930729
			US 1994-254823 A2	19940613

NZ 1994-264116 A1 19940728

OTHER SOURCE(S): MARPAT 128:321569

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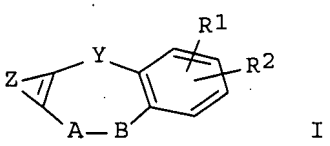

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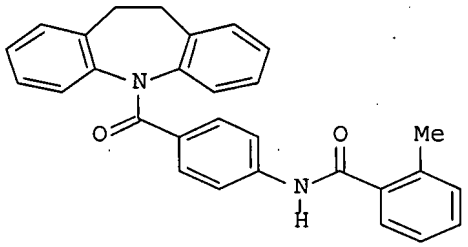


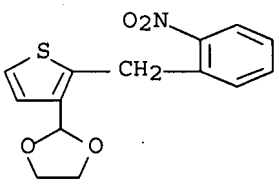
II

AB The title compds. [I; Y = a bond; AB = (CH2)2N(R3); R1 = H, halo, OH, etc.; R2 = H, halo, OH, etc.; R1R2 = methylenedioxy, ethylenedioxy; R3 = C(O)Ar (wherein Ar = (un)substituted Ph, thienyl, etc.); Z = (un)substituted fused benzo, thiazole, etc.], which exhibit antagonistic activity at V1 and/or V2 receptors, in vivo vasopressin antagonist activity, and antagonistic activity at oxytocin receptors, and therefore useful in treating diseases characterized by excess renal reabsorption of water such as congestive heart failure, nephrotic syndrome, hyponatremia, coronary vasospasm, cardiac ischemia, liver cirrhosis, brain edema, cerebral ischemia, or cerebral hemorrhage-stroke, were prepd. Thus, reaction of 4-[(2-methylbenzoyl)amino]benzoyl chloride with 10,11-dihydro-5H-dibenz[b,f]azepine in the presence of 4-(dimethylamino)pyridine in pyridine afforded the title compd. II which showed IC50 of 2.5 .mu.M against rat hepatic V1 receptors binding and IC50 of 0.86 .mu.M against rat kidney medullary V2 receptors binding.

IT 167770-26-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of tricyclic benzazepine vasopressin antagonists)

RN 167770-26-5 CAPLUS

CN 1,3-Dioxolane, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:219347 CAPLUS Full-text

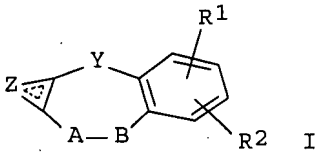
DOCUMENT NUMBER: 128:257347

TITLE: Tricyclic benzazepine oxytocin and vasopressin antagonists

INVENTOR(S): Albright, Jay Donald; Du, Xuemei
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 109 pp., Cont.-in-part of U.S. 5,512,563.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5736538	A	19980407	US 1996-638059	19960425
US 5512563	A	19960430	US 1994-254823	19940613
NZ 299340	A	20000825	NZ 1994-299340	19940728
PRIORITY APPLN. INFO.:			US 1993-100003 B2	19930729
			US 1994-254823 A2	19940613
			NZ 1994-264116 A1	19940728

OTHER SOURCE(S): MARPAT 128:257347
GI



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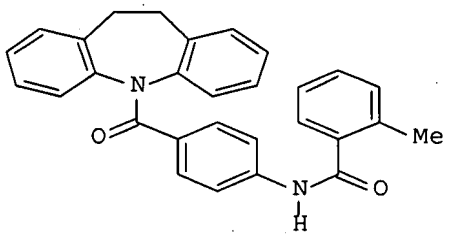


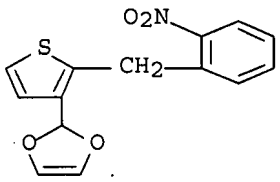
II

AB This invention relates to title compds. I wherein: Y = e.g., (CH2)n, O, S wherein n is an integer from 0-2; A-B is (CH2)mNR3 or NR3(CH2)m , wherein m is an integer from 1-2, provided that when Y is (CH2)n and n=2, m may also be zero and when n is zero, m may also be three, provided also that when Y is (CH2)n and n is 2, m may not also be two; R1 = e.g., H, halo, OH; R2 = e.g., H, halo, OH; R3 is the moiety COAr where Ar is selected from, e.g., substituted Ph, (un)substituted 5-indolyl; the arom. Z ring represents, e.g., fused (un)substituted Ph, 5- or 6-membered atom. heterocycle, that exhibit antagonist activity at V1 and/or V2 receptors and exhibit in vivo vasopressin antagonist activity, methods for using such compds. in treating diseases characterized by excess renal reabsorption of water, and processes for prepg. such compds. I are also antagonists of the peptide hormone oxytocin and are useful in the control of premature birth. Thus, e.g., acylation of 6,11-dihydro-5H- dibenz[b,e]azepine (prepn. given) with 4-[(2-methylbenzoyl)amino]benzoyl chloride (prepn. given) afforded N-[4-[(6,11-dihydro-5H-dibenz[b,e]azepin- 5-yl)carbonyl]phenyl]-2-methylbenzamide (II) which exhibited binding to rat hepatic V1 receptors and rat kidney medullary V2 receptors with IC50 = 0.15 and 0.068 .mu.M, resp., and oxytocin receptor binding with IC50 = 2.9 .mu.M.

IT 178448-00-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tricyclic benzazepine oxytocin and vasopressin antagonists)

RN 178448-00-5 CAPLUS
CN 1,3-Dioxole, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX

NAME)

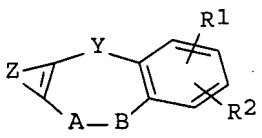


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

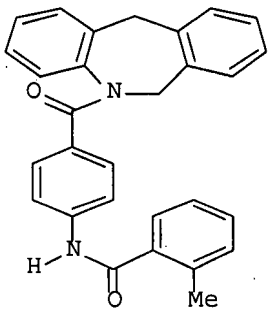
L6 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:13962 CAPLUS Full-text
DOCUMENT NUMBER: 128:75393
TITLE: Preparation of tricyclic benzazepines as vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Reich, Marvin Fred
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: PCT Int. Appl., 289 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9747624	A1	19971218	WO 1997-US9548		19970603
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, TJ, TM					
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9732964	A	19980107	AU 1997-32964		19970603
PRIORITY APPLN. INFO.:			US 1996-663400	A	19960613
			WO 1997-US9548	W	19970603

OTHER SOURCE(S): MARPAT 128:75393
GI



I



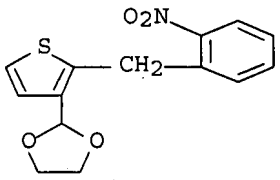
II

AB The title compds. [I; Y = a bond, CH2; AB = (CH2)2NR3, NR3(CH2)2; R1 = H, halo, OH, etc.; R2 = H, halo, OH, etc.; R1R2 = methylenedioxy, ethylenedioxy; R3 = C(O)Ar; Ar = (un)substituted Ph, 5-indolyl, thienyl, etc.; Z = (un)substituted fused pyrazole, benzene, etc.] and their salts which exhibit vasopressin antagonist activity and are useful in treating diseases characterized by excess renal reabsorption of water, were prepd. Thus, reaction of 4-[(2-methylbenzoyl)amino]benzoyl chloride with 6,11-dihydro-5H-dibenz[b,e]azepine in the presence of Et3N in THF afforded the title compd. II which showed IC50 of 0.15 .mu.M against rat hepatic V1 receptor binding and IC50 of 0.068 .mu.M against rat kidney medullary V2 receptor binding. Compd. II also showed 73% inhibition of oxytocin receptor binding at 10 .mu.M.

IT 167770-26-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of tricyclic benzazepines as vasopressin antagonists)

RN 167770-26-5 CAPLUS

CN 1,3-Dioxolane, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:772293 CAPLUS Full-text

DOCUMENT NUMBER: 128:48246

TITLE: Preparation of tricyclic benzazepines as vasopressin antagonists

INVENTOR(S): Albright, Jay Donald; Reich, Marvin Fred

PATENT ASSIGNEE(S): American Cyanamid Co., USA

SOURCE: U.S., 103 pp., Cont.-in-part of U.S. Ser. No. 639,014.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

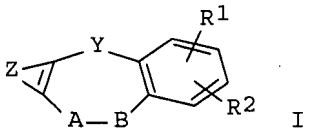
FAMILY ACC. NUM. COUNT: 10

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5693635	A	19971202	US 1996-662546	19960613
US 5512563	A	19960430	US 1994-254823	19940613
NZ 299340	A	20000825	NZ 1994-299340	19940728
US 5869483	A	19990209	US 1996-639014	19960424
WO 9747625	A1	19971218	WO 1997-US9549	19970603
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9732965	A	19980107	AU 1997-32965	19970603
PRIORITY APPLN. INFO.:			US 1993-100003 B2	19930729
			US 1994-254823 A2	19940613
			US 1996-639014 A2	19960424
			NZ 1994-264116 A1	19940728
			US 1996-662546 A	19960613
			WO 1997-US9549 W	19970603

OTHER SOURCE(S): MARPAT 128:48246

GI



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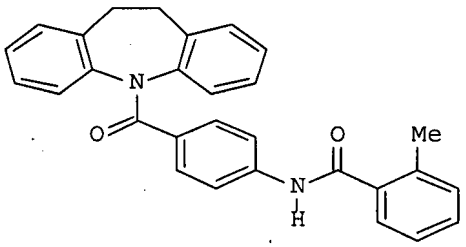


II

AB The title compds. [I; Y = a bond; AB= (CH2)2NR3, NR3(CH2)2; R1 = H, halo, OH, etc.; R2 = H, halo, OH, etc.; R1R2 = methylenedioxy, ethylenedioxy; R3 = COAr (wherein Ar = substituted Ph); Z with two carbon atoms attached represents a (un)substituted fused thiophene ring, Ph, etc.] which exhibit antagonist activity at V1 and/or V2 receptors, in vivo vasopressin antagonist activity, and also antagonist activity at oxytocin receptors, and are useful in treating diseases characterized by excess renal reabsorption of water, were prepd. Thus, reaction of 4-[(2-methylbenzoyl)amino]benzoyl chloride with 10,11-dihydro-5H- dibenz[b,f]azepine in the presence of NaH and 4-(dimethylamino)pyridine in pyridine afforded II which showed IC50 of 2.5 .mu.M against rat hepatic V1 receptor binding and IC50 of 0.86 .mu.M against rat kidney medullary V2 receptor binding.

IT 167770-26-5P

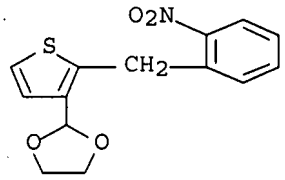
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of tricyclic benzazepines as vasopressin antagonists)

RN 167770-26-5 CAPLUS

CN 1,3-Dioxolane, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX

NAME)



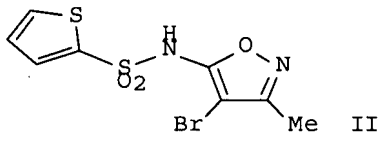
L6 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:761669 CAPLUS Full-text
DOCUMENT NUMBER: 126:31342
TITLE: Preparation of N-isoxazolylthiophenesulfonamides and analogs as endothelin receptor antagonists
INVENTOR(S): Chan, Ming Fai; Raju, Bore Gowda; Kois, Adam; Verner, Erik Joel; Wu, Chengde; Castillo, Rosario Silverstre; Yalamoori, Venkatachalapathi; Balaji, Vitukudi Narayanaiyenga
PATENT ASSIGNEE(S): Texas Biotechnology Corporation, USA
SOURCE: PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9631492	A1	19961010	WO 1996-US4759	19960404
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
US 5594021	A	19970114	US 1995-477223	19950606
AU 9655367	A	19961023	AU 1996-55367	19960404
AU 711968	B2	19991028		
EP 819125	A1	19980121	EP 1996-912600	19960404
EP 819125	B1	20030618		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
BR 9604875	A	19980519	BR 1996-4875	19960404
JP 11507015	T	19990622	JP 1996-530524	19960404
JP 3233642	B2	20011126		
NZ 306734	A	20000128	NZ 1996-306734	19960404
HU 9802034	A2	20000328	HU 1998-2034	19960404
AT 243203	T	20030715	AT 1996-912600	19960404
PL 186854	B1	20040331	PL 1996-322707	19960404
US 5962490	A	19991005	US 1996-721183	19960927
NO 9704577	A	19971204	NO 1997-4577	19971003
NO 315607	B1	20030929		
MX 9707630	A	20000331	MX 1997-7630	19971003
US 2001021714	A1	20010913	US 1997-913331	19971107

US 6342610	B2	20020129			
HK 1001769	A1	20040130	HK 1998-100844		19980205
US 6331637	B1	20011218	US 1999-274280		19990322
AU 9935803	A	19990916	AU 1999-35803		19990622
AU 726595	B2	20001116			
US 2002091272	A1	20020711	US 2001-11610		20011105
US 6632829	B2	20031014			
PRIORITY APPLN. INFO.:			US 1995-416199	A	19950404
			US 1995-417075	A	19950404
			US 1995-477223	A	19950606
			US 1987-100865	A2	19870925
			US 1990-416199	A2	19900515
			US 1993-65202	B2	19930520
			US 1993-100125	B2	19930730
			US 1993-100565	B2	19930730
			US 1993-142159	A2	19931021
			US 1993-142552	A2	19931021
			US 1993-142631	B2	19931021
			US 1994-222287	A2	19940405
			US 1994-247072	A2	19940520
			AU 1996-55367	A	19960404
			WO 1996-US4759	W	19960404
			US 1996-721183	A1	19960927
			US 1997-938325	A3	19970926

OTHER SOURCE(S): MARPAT 126:31342

GI



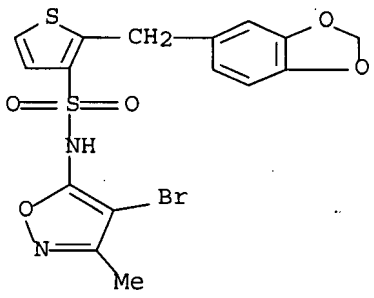
II

AB R2SO2NHR1 [I; R1 = (hetero)aryl; R2 = (un)substituted biphenylyl, -2- or -3-furyl, -thienyl, -pyrrolyl] were prepd. Thus, 5-amino-4-bromo-3-methylisoxazole (prepn. given) was amidated by thiophene -2-sulfonyl chloride to give title compd. II. Data for biol. activity of I were given.

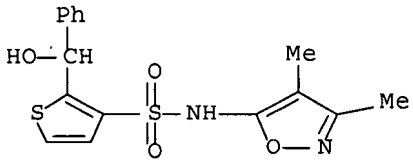
IT 184035-71-0P 184035-86-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-isoxazolylthiophenesulfonamides and analogs as endothelin receptor antagonists)

RN 184035-71-0 CAPLUS

CN 3-Thiophenesulfonamide, 2-(1,3-benzodioxol-5-ylmethyl)-N-(4-bromo-3-methyl-5-isoxazolyl)- (CA INDEX NAME)

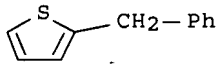


RN 184035-86-7 CAPLUS
CN 3-Thiophenesulfonamide, N-(3,4-dimethyl-5-isoxazolyl)-2-(hydroxyphenylmethyl)- (9CI) (CA INDEX NAME)

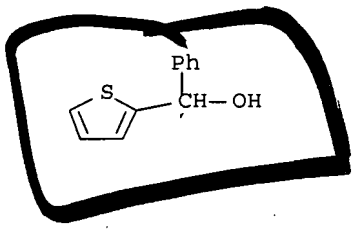


IT 13132-15-5P, 2-Benzylthiophene 26059-21-2P, .alpha.-(2-Thienyl)benzyl alcohol 184040-60-6P 184040-62-8P 184041-07-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-isoxazolylthiophenesulfonamides and analogs as endothelin receptor antagonists)

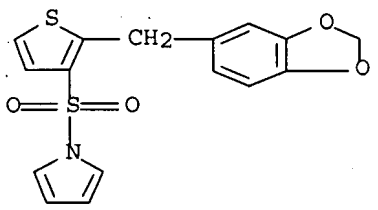
RN 13132-15-5 CAPLUS
CN Thiophene, 2-(phenylmethyl)- (CA INDEX NAME)



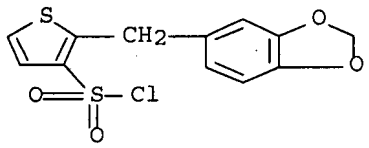
RN 26059-21-2 CAPLUS
CN 2-Thiophenemethanol, .alpha.-phenyl- (CA INDEX NAME)



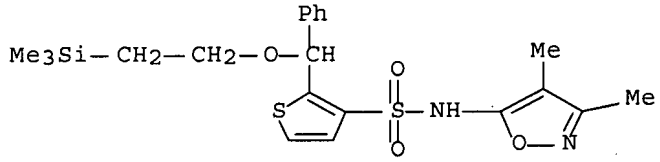
RN 184040-60-6 CAPLUS
CN 1H-Pyrrole, 1-[[2-(1,3-benzodioxol-5-ylmethyl)-3-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 184040-62-8 CAPLUS
CN 3-Thiophenesulfonyl chloride, 2-(1,3-benzodioxol-5-ylmethyl)- (9CI) (CA INDEX NAME)

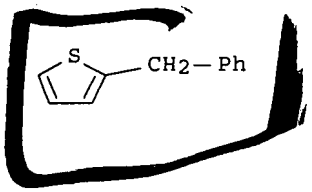


RN 184041-07-4 CAPLUS
CN 3-Thiophenesulfonamide, N-(3,4-dimethyl-5-isoxazolyl)-2-[phenyl[2-(trimethylsilyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:644491 CAPLUS Full-text
DOCUMENT NUMBER: 125:300734
TITLE: Pyrolytic chemistry of thenyl benzoates
AUTHOR(S): Chen, Ping-Shu; Chou, Chin-Hsing
CORPORATE SOURCE: Dep. of Chemistry, National Sun Yat-Sen Univ., Kaohsiung, 80424, Taiwan
SOURCE: Tetrahedron (1996), 52(43), 13615-13622
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flash vacuum pyrolysis of 2- and 3-thenyl benzoates at temps. in the range 550-750.degree. and ca. 10-2 torr gave several radical-derived products. The mechanism of formation of these pyrolysis products is proposed to involve 2- and 3-thenyl and Ph radicals.
IT 13132-15-5P, 2-(Phenylmethyl)thiophene
RL: SPN (Synthetic preparation); PREP (Preparation)

(pyrolytic chem. of thenyl benzoates)
RN 13132-15-5 CAPLUS
CN Thiophene, 2-(phenylmethyl)- (CA INDEX NAME)



L6 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:323956 CAPLUS Full-text
DOCUMENT NUMBER: 125:86517
TITLE: Tricyclic benzazepine oxytocin and vasopressin antagonists
INVENTOR(S): Albright, Jay D.; Sum, Fuk Wah; Du, Xuemei
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 95 pp., Cont.-in-part of U.S. Ser. No. 100,003, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5512563	A	19960430	US 1994-254823	19940613
EP 640592	A1	19950301	EP 1994-111040	19940715
EP 640592	B1	19981230		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 175198	T	19990115	AT 1994-111040	19940715
ES 2125377	T3	19990301	ES 1994-111040	19940715
SK 281194	B6	20010118	SK 1994-880	19940720
IL 110436	A	20031210	IL 1994-110436	19940725
FI 9403542	A	19950130	FI 1994-3542	19940728
FI 108433	B1	20020131		
NO 9402817	A	19950130	NO 1994-2817	19940728
NO 308601	B1	20001002		
AU 9468776	A	19950209	AU 1994-68776	19940728
AU 676737	B2	19970320		
ZA 9405604	A	19950309	ZA 1994-5604	19940728
JP 07179430	A	19950718	JP 1994-195886	19940728
JP 3630449	B2	20050316		
HU 71548	A2	19951228	HU 1994-2223	19940728
HU 221017	B1	20020729		
RU 2149160	C1	20000520	RU 1994-27580	19940728
NZ 299340	A	20000825	NZ 1994-299340	19940728
CN 1106802	A	19950816	CN 1994-108768	19940729
CN 1064354	B	20010411		
PL 181918	B1	20011031	PL 1994-304496	19940729
TW 402592	B	20000821	TW 1994-83108599	19940916
US 5739128	A	19980414	US 1996-637058	19960424
US 5869483	A	19990209	US 1996-639014	19960424
US 5686445	A	19971111	US 1996-637908	19960425
US 5736538	A	19980407	US 1996-638059	19960425
US 5747487	A	19980505	US 1996-638067	19960425
US 5760031	A	19980602	US 1996-637911	19960425

US 5693635	A	19971202	US 1996-662546	19960613
US 5854236	A	19981229	US 1997-834706	19970401
US 5834461	A	19981110	US 1997-874314	19970613
US 5843952	A	19981201	US 1997-889858	19970708
US 5786353	A	19980728	US 1997-893497	19970711
HK 1011362	A1	20010727	HK 1998-112373	19981127
FI 2001001100	A	20010525	FI 2001-1100	20010525
FI 111077	B1	20030530		
FI 2001001101	A	20010525	FI 2001-1101	20010525
FI 111075	B1	20030530		
FI 2001001102	A	20010525	FI 2001-1102	20010525
FI 111076	B1	20030530		

PRIORITY APPLN. INFO.:

US 1993-100003	B2 19930729
US 1994-254823	A2 19940613
NZ 1994-264116	A1 19940728
US 1996-637058	A3 19960424
US 1996-639014	A2 19960424
US 1996-637908	A3 19960425
US 1996-663400	B1 19960613

OTHER SOURCE(S): MARPAT 125:86517

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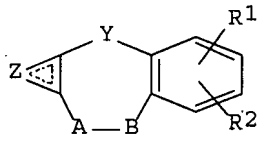
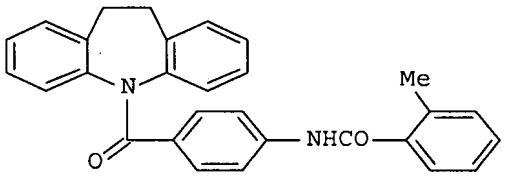


I



II

AB This invention relates to title compds. I wherein: Y = e.g., (CH2)n, O, S wherein n is an integer from 0-2; A-B is (CH2)mNR3 or NR3(CH2)m , wherein m is an integer from 1-2, provided that when Y is (CH2)n and n=2, m may also be zero and when n is zero, m may also be three, provided also that when Y is (CH2)n and n is 2, m may not also be two; R1 = e.g., H, halo, OH; R2 = e.g., H, halo, OH; R3 is the moiety COAr where Ar is selected from, e.g., substituted Ph, (un)substituted 5-indolyl; the arom. Z ring represents, e.g., fused (un)substituted Ph, 5- or 6-membered atom. heterocycle, that exhibit antagonist activity at V1 and/or V2 receptors and exhibit in vivo vasopressin antagonist activity, methods for using such compds. in treating diseases characterized by excess renal reabsorption of water, and processes for prepg. such compds. I are also antagonists of the peptide hormone oxytocin and are useful in the control of premature birth. Thus, e.g., acylation of 6,11-dihydro-5H- dibenz[b,e]azepine (prepn. given) with 4-[(2-methylbenzoyl)amino]benzoyl chloride (prepn. given) afforded N-[4-[(6,11-dihydro-5H-dibenz[b,e]azepin- 5-yl)carbonyl]phenyl]-2-methylbenzamide (II) which exhibited binding to rat hepatic V1 receptors and rat kidney medullary V2 receptors with IC50 = 0.15 and 0.068 .mu.M, resp., and oxytocin receptor binding with IC50 = 2.9 .mu.M.

IT 178448-00-5P

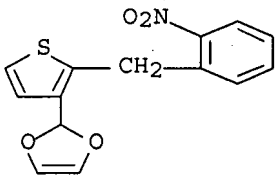
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(tricyclic benzazepine oxytocin and vasopressin antagonists)

RN 178448-00-5 CAPLUS

CN 1,3-Dioxole, 2-[2-[(2-nitrophenyl)methyl]-3-thienyl]- (9CI) (CA INDEX

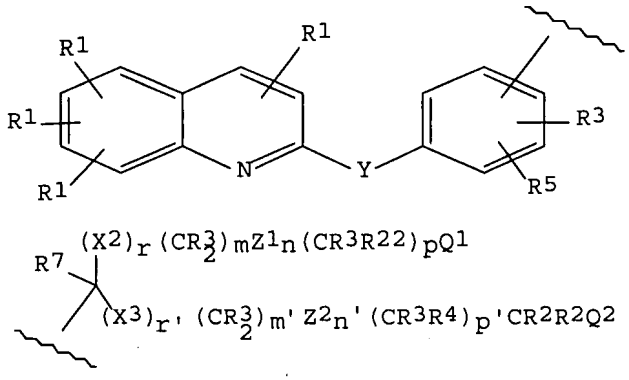
NAME)



L6 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:705723 CAPLUS Full-text
DOCUMENT NUMBER: 124:8639
TITLE: Saturated hydroxyalkylquinoline acids as leukotriene antagonists
INVENTOR(S): Belley, Michel L.; Leger, Serge; Roy, Patrick; Xiang, Yi B.; Labelle, Marc
PATENT ASSIGNEE(S): Merck Frosst Canada, Inc., Can.
SOURCE: U.S., 29 pp. Cont.-in-part of U.S. Ser. No. 596,844, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5428033	A	19950627	US 1991-774396	19911010
CA 2053216	A1	19920413	CA 1991-2053216	19911010
CA 2053216	C	20030408		
HU 61980	A2	19930329	HU 1991-3216	19911010
FI 9104797	A	19920413	FI 1991-4797	19911011
NO 9104002	A	19920413	NO 1991-4002	19911011
AU 9185796	A	19920416	AU 1991-85796	19911011
AU 639611	B2	19930729		
CN 1061408	A	19920527	CN 1991-110823	19911011
ZA 9108120	A	19920624	ZA 1991-8120	19911011
JP 06206868	A	19940726	JP 1991-331111	19911014
JP 2538155	B2	19960925		

PRIORITY APPLN. INFO.: US 1990-596844 B2 19901012
OTHER SOURCE(S): CASREACT 124:8639; MARPAT 124:8639
GI



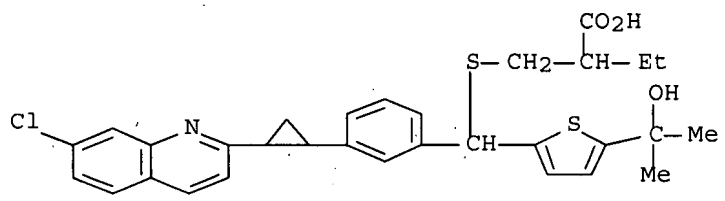
I

AB Quinolines I [R1 = e.g., H, halo, CF3; R2 = e.g., lower alkyl, lower alkenyl, lower alkynyl; R3 is H or R2; R4 = e.g., halo, NO2, CN; R5 = e.g., H, halo, NO2; R7 = H or C1-4 alkyl; R16 = H, C1-4 alkyl, OH; R22 = R4, CHR7OR3 or CHR7SR2; X2 and X3 are independently O, S, SO, SO2, or CR3R16 with the proviso that at least one is S or SO2; Y = e.g., CR3R3CR3R3; Z1 and Z2 are independently HET(R3R5); HET is the diradical of a benzene, a pyridine, a furan, or a thiophene; Q1 = e.g., CO2R3, 1H(or 2H)-tetrazol-5-yl; Q2 = e.g., OH; m and m' are independently 0-8; n and n' are independently 0 or 1, p and p' are independently 0-8; m+n+p is 1-10 when r is 1 and X2 is O, S, S(O), or SO2; m+n+p is 0-10 when r is 1 and X2 is CR3R16; m+n+p is 0-10 when r is 0; m'+n'+p' is 0-10; r and r' are independently 0 or 1; and the pharmaceutically acceptable salts thereof] are leukotriene antagonists and inhibitors of leukotriene biosynthesis (no data). These compds. are useful as anti-asthmatic, anti-allergic, anti-inflammatory, and cytoprotective agents. They are also useful in treating angina, cerebral spasm, glomerular nephritis, hepatitis, endotoxemia, uveitis, and allograft rejection. Pharmaceutical formulations were given. Thus, e.g., reaction of 3-mercapto-2-methylpropanoic acid (prepn. given) with Me 2-[3-[3-[2-(7-chloro-2-quinolinyl)ethyl]phenyl]-2-propenyl]benzoate followed by treatment with MeMgBr and NaOH afforded the Na propanoate II.

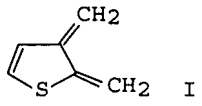
IT 142119-63-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(satd. hydroxyalkylquinoline acids as leukotriene antagonists)

RN 142119-63-9 CAPLUS

CN Butanoic acid, 2-[[[[3-[2-(7-chloro-2-quinolinyl)cyclopropyl]phenyl][5-(1-hydroxy-1-methylethyl)-2-thienyl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

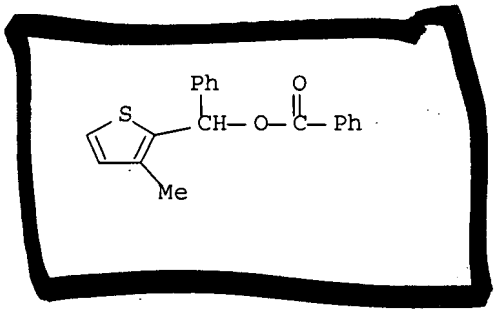


L6 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:33963 CAPLUS Full-text
DOCUMENT NUMBER: 104:33963
TITLE: Preparation of 2,3-dimethylene-2,3-dihydrothiophenes by the flash vacuum pyrolysis of substituted thiophenemethyl benzoates
AUTHOR(S): Huang, Y. J.
CORPORATE SOURCE: Ames Lab., Ames, IA, USA
SOURCE: Report (1984), IS-T-1139; Order No. DE85007077, 66 pp. Avail.: NTIS
From: Energy Res. Abstr. 1985, 10(8), Abstr. No. 13937
DOCUMENT TYPE: Report
LANGUAGE: English
GI



I

AB Flash vacuum pyrolysis of 3-methyl-2-thenyl benzoate and 2-methyl-3-thenyl benzoate provides a convenient method for the generation of the previously unknown 2,3-dimethylene-2,3-dihydrothiophene (I) and consequently the isolation of its [4 + 2] spirodimer as the major product. The consistently low yield (.apprx.20%) of the spiro-dimer and the inability to trap I intermolecularly clearly indicate that I is an extremely reactive species which dimerizes and polymerizes at very low temps. In the pyrolysis of 3-methyl-.alpha.-phenyl-2-thenyl benzoate, the 2,3-dimethylene-2,3-dihydrothiophene moiety is cleanly trapped by its Ph substituent and affords naphtho[2,3-b] thiophene as the major product.
IT 99646-80-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(flash vacuum pyrolysis of)
RN 99646-80-7 CAPLUS
CN 2-Thiophenemethanol, 3-methyl-.alpha.-phenyl-, benzoate (9CI) (CA INDEX NAME)



L6 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:447734 CAPLUS Full-text
DOCUMENT NUMBER: 65:47734
ORIGINAL REFERENCE NO.: 65:8922f-h,8923a-h,8924a-h,8925a-h
TITLE: Substituted 1,3,8-triazaspiro[4.5]decanes
INVENTOR(S): Janssen, Paul A. J.
PATENT ASSIGNEE(S): Janssen Pharmaceutica NV

SOURCE: 37 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3238216		19660301	US 1963-289443	19630620
PRIORITY APPLN. INFO.:			US	19630620

GI For diagram(s), see printed CA Issue.

AB Condensation of a 4-piperidone or 4-hydroxypiperidine alkali metal sulfide, protected at the N, with a primary amine and an alkali metal cyanide causes simultaneous introduction of the nitrile and secondary amino groups in the piperidyl ring at the 4-position with production of I. The nitrile function is converted to the amide (Ia) by acid hydrolysis. Thus, 95 parts 1-benzyl-4-oxopiperidine, 50 parts cyclohexylamine, 50 parts concd. HCl, 65 parts EtOH, and 60 parts H2O are mixed while being stirred and cooled. A soln. of 32.5 parts KCN in 40 parts H2O is added dropwise with stirring overnight to yield I (R = cyclohexyl) (Ib), m. 82-3.degree.. Ib (20 parts) is added slowly to 110 parts of concd. H2SO4 in 15 min. The temp. rises to 80.degree., the mixt. is stirred 1 hr. and poured into excess ammoniacal ice-water to give Ia, m. 138.8-9.6.degree.. The following V were similarly prepd. (R, m.p., and m.p. Ia given): Ph, 145-6.degree., 187-88.degree., Me, 63-4.degree., 156-7.degree.; 3-MeC6H4, 95-7.degree., 115-22.degree.; 3-MeOC6H4, 97-8.degree., 130-1.degree.; 4-MeC6H4, 112-15.degree., 166-7.5.degree.; 4-ClC6H4, 157-9.degree., 172-3.degree.; 2-MeC6H4, 117-20.degree., 126-8.degree.; Bu, 75-7.degree., 114-18.degree.; 4-MeOC6H4, 110-17.degree., 131-4.degree.; Et, 56-7.degree., 113.6-15.degree.; iso-Pr, 64-7.degree., 118-20.degree.; Pr, -, 128-31.degree.. Cyclization of Ia is effected by treatment with formamide to yield II if the secondary amino group attached to the piperidine ring is alkyl substituted or the satd. analog (III) of II, if aryl substituted. However, with the Et group III is obtained. Reaction of Ia with (EtO)3CH also yields II. Thus, a mixt. of 6.2 parts 1-benzyl-4-carbamoyl-4-anilinopiperidine, 3.1 parts Ac2O, and 40 parts toluene is stirred and refluxed 16 hrs. to yield 1-phenyl-2-methyl-4-oxo-8- benzyl-1,3,8-triazaspiro[4.5]dec-2-ene, m. 211.5-14.5.degree.. The following II were similarly prepd. (R2 = H, R3 = benzyl) (R1 and m.p. given): Me, 178-9.5.degree.; Ph, 171-3.degree.; cyclohexyl, 209-11.degree.; iso-Pr, 193-4.degree.; Pr, 147-57.degree.; Bu, 265-7.5.degree. (2 HCl). The following III were also prepd. (R2 = H, R3 = benzyl) (R1 and m.p. given): Ph, 232-8.5.degree.; 3-methylphenyl, 204-9.degree.; 4-methylphenyl, 221-3.degree.; 4-chlorophenyl, 210-15.degree.; 3-methoxyphenyl, 212-14.degree.; 3-methylphenyl, 151-61.degree.; 4-methoxyphenyl, 184-5.degree.; Et, 139-45.degree.. Also prepd. were III (R1 = Ph, R2 = H) (R3 and m.p. given): 3-(4-fluorobenzoyl)propyl, 242-3.degree. (HCl salt); 3-(4- fluorophenyl)propyl, 205-6.5.degree. (picrate). Ring closure of Ia is alternatively accomplished by treatment with an acylating agent leading to II, II can be reduced to III with LiAlH4 or NaAlH4. Thus, to a mixt. of 0.6 part LiAlH4, 48 parts benzene, and 24 parts tetrahydrofuran (THF) is added 5.4 parts 1-phenyl-2-methyl-4-oxo-8-benzyl-1,3,8-triazaspiro[4.5]dec- 2-ene and the mixt. refluxed 20 hrs. to give dl-1-phenyl-2-methyl-4-oxo-8- benzyl-1,3,8-triazaspiro[4.5]decane, m. 150-1.8.degree.. For 2-methyl substituted dec-2-enes, debenzylation by means of H activated by Pd-C catalyst can be carried out before or after satn. of the cyclic double bond. If the .alpha.-position of II is unsubstituted, satn. of the ring precedes debenzylation. Thus, a mixt. of 14.9 parts 1-phenyl-2-methyl-4- oxo-8-benzyl-1,3,8-triazaspiro [4.5]dec-2-ene (IV) and 160 parts 95% EtOH is debenzylated at normal pressure and 37-9.degree. in the presence of 5 parts 10% Pd-C to yield 1-phenyl-2-methyl-4-oxo-1,3,8-triazaspiro-[4.5] dec-2-ene, m. 197.4-205.degree.. The following III were similarly prepd. (R3 = H) (R1, R2, and m.p. given): Me, H, 200-3.degree. (HCl); cyclohexyl, H, 205-

20.degree. (2HCl); Ph, Me (dl), 196-7.5.degree.; iso-Pr, H, 158-61.degree.; Pr, H, 212-13.degree. (decompn.) (2HCl); Bu, H, 110-227.degree. (decompn.) (2HCl). A mixt. of 5 parts 1-phenyl-4-oxo-8-benzyl-1,3,8-triazaspiro[4,5]decane, 10 parts Ac2O, and 40 parts PhMe is refluxed 15 hrs. to give 1-phenyl-3-acetyl-4-oxo-8-benzyl- 1,3,8-triazaspiro[4.5]decane, m. 128-30.degree.. The following V (R1 = Ph) were similarly prepd. (R2, R3, and m.p. given): Me, benzyl, 136-84.degree.; CH2OH, benzyl, 169-70.degree.; Et, benzyl, 234-8.degree.; Ac, 3-cyano-3,3-diphenylpropyl, 219-20.5.degree.; 2-cyanoethyl, benzyl, 218-19.degree.; Ac, 3-(4-fluorobenzyl)propyl (X), 188-213.degree.; propionyl, X, 87-8.degree.; propionyl, benzyl, 110-11.degree.; Ac, 2-(benzo-1,4-dioxanyl)methyl (Y), 140.degree. (decompn.) (HCl); propionyl, Y (dl), 141-7.degree.; cyclopropylcarbonyl, Y (dl), 140-96.degree. (decompn.), Bz, Y, 188.5-90.degree.; propionyl, 4-(4-fluorophenyl)-4- phenylbutyl, 102.5-103.degree.; propionyl, 4,4-bis(4-fluorophenyl)butyl, 113-14.degree.; Me, Y (dl), 227-8.degree.; 2-(ethylcarbonyl)ethyl, Y (dl), 93-114.degree.; benzyl, Y (dl), 230-2.degree. (HCl); CH2OH, Y (dl), 169-75.degree.; methoxylmethyl, Y (dl), 138-83.degree. (decompn.) (oxalate); 2-cyanoethyl, Y, 181-7.degree. (oxalate); 2-carbamoylethyl, Y (dl), 175-84.degree. (HCl); 3-methoxymethyl, benzyl, 105.5-10.degree.. To a mixt. of 3.9 parts 1-phenyl-4-oxo-1,3,8-triazaspiro[4.5]decane, 3.2 parts Na2CO3 and a few crystals of KI in 160 parts 4-methyl-2-pentenone is added dropwise 2.8 parts 1-chloro-2-phenylethane in 40 parts 4-methyl-2-pentenone and refluxed 48 hrs. to give 1-phenyl-4-oxo-8-(2-phenylethyl)-1,3,8-triazaspiro[4.5]-decane, m. 198.6-201.degree.. The following III (R2 = H) are similarly prepd. (R1, R3, and m. given): Ph, 3-cyano-3,3-diphenylpropyl, 178-84; Ph, 2-phenoxyethyl, 214-17.5.degree.; Ph, 2-(1,4-benzodioxanyl)methyl, 215.8-18.degree.; Ph, 3-phenoxypropyl, 154.2-56.degree.; Ph, 2-thienylmethyl, 220-3.degree.; Ph, 4-fluorobenzyl, 224-34.degree.; Ph, 4-methylbenzyl, 182.6-5.4.degree.; Ph, 2-pyridylmethyl, 195-201.degree.; Ph, 2,5-dimethylbenzyl, 206-8.4.degree.; Ph, 3,3-diphenyl-4-oxohexyl, 226-8.degree.; Ph, 2-methylbenzyl, 217-19.degree.; Ph, 3-methylbenzyl, 220-5.degree.; Ph, 3-phenylpropyl, 169.6-70.8.degree.; Me, 3-cyano-3,3-diphenylpropyl, 117.4-21; 3-methylphenyl, 3-cyano-3,3-diphenylpropyl, 206-12.degree.; 4-methylphenyl, 3-cyano-3,3-diphenylpropyl, 205-11.degree.; cyclohexyl, 3-cyano-3,3-diphenylpropyl, 172.5-75.degree.; Ph, 2-(2- hydroxyethoxy)ethyl, 198-234.degree.; 4-methylphenyl, 2-phenoxyethyl, 177-7.5.degree.; Me, 2-phenoxyethyl, 109-13.degree.; cyclohexyl, 2-phenoxyethyl, 161-2.5.degree.; Ph, cinnamyl, 171-2.degree.; Ph, 4-phenoxybutyl, 85-112.degree.; Ph, 3,3-diphenylpropyl, 247-51.degree. (HCl); Ph, 3,3-diphenyl-3-hydroxypropyl, 226-31.5.degree.; (dl) Ph, 2-(1,4-benzoyldioxanyl)ethyl, 142-202.degree. (decompn.) (HCl); Ph, 3-(4-fluorobenzoyl)propyl, 190-4.degree.; Ph, 3-benzoylpropyl, 174-8.degree.; Ph, 4-oxo-4-(2-thienyl)butyl, 173-7.degree.; 3-methylphenyl, X, 181-3.degree.; 4-methylphenyl, X, 178-81.degree.; Ph, 3-(4-chlorobenzoyl)propyl, 202-4.degree.; Me, X, 204-12.degree. (2HCl); (dl) Ph, X (R2 = Me), 148-50.degree.; 4-methoxyphenyl, X, 163-5.degree.; Ph, Pr, 190.6-3.8.degree.; iso-Pr, X, 212.6-14.degree., (decompn.) (2HCl); (dl) Ph, 4-(4-fluorophenyl)-4-hydroxybutyl, 175.5-77.degree.; Ph, 3-(4-methoxybenzyl)propyl, 178.4-80.degree.; cyclohexyl, X, 206-15.degree. (decompn.) (2HCl); Ph, 4-benzoylbutyl; 169.5-84.degree.; Ph, H, 168-76.degree.; 4-methylphenyl, H, 190-1.4.degree.; 3-methylphenyl, H, 189.8-90.8.degree.; 4-methoxyphenyl, H, 195-6.degree.; Ph, iso-Pr, 185-90.degree.; Ph, Bu, 178.6-80.degree.; Ph, Am, 189.8-90.8.degree., Ph, heptyl, 165-6.6.degree.; Ph, octyl, 167-8.degree.; Ph, nonyl, 169.5-70.degree.; (dl) iso-Pr, Y, 156-7.degree.; (dl) Bu, Y, 185-8.degree. (2HCl); (dl) Ph, Y, 247.5-49.degree.; (dl) Ph, 2-(7-bromo-1,4-benzodioxanyl)methyl, 199-208.degree.; (dl) Ph, 2-(1,4-benzodioxanyl)propyl, 188-93.6.degree.; (dl) Ph, 1-phenylpropyl, 198.5-201.degree.; (dl) Ph, 1-(4-methylphenyl)ethyl, 162-4.degree.; (dl) Ph, 1-(4-methylphenyl)propyl, 199-201.5.degree.; (dl) Ph, 1-(4-fluorophenyl)ethyl, 232-8.degree.; (dl) Ph, 1-(4-fluorophenyl)propyl, 232-8.degree.; (dl)Ph, 1-(4- chlorophenyl)propyl, 198.5-202.degree.; Ph, 2-(4-methylphenyl)ethyl, 233.5-36.degree.; Ph, 2-(4-

methoxyphenyl)ethyl, 204-5.degree.; Ph, 2-(4-fluorophenyl)ethyl, 201.5-3.5.degree.; Ph, 4-phenylbutyl, 188.5-90.degree., Ph, 4-(4-fluorophenyl)butyl, 180-1.degree.; (dl) Ph, 2-phenylbutyl, 176-9.degree.; (dl) Ph, 3-phenylbutyl, 166.5-7.5.degree.; (dl) Ph, 2-methyl-3-phenylpropyl, 190.5-93.degree.; (dl) Ph, 1-methyl-3-phenylpropyl, 164-5.5.degree.; (dl) Ph, 4-phenylpentyl, 121.5-5.5.degree.; (dl) Ph, 4-(4-methylphenyl)pentyl, 133-5.degree.; (dl) Ph, 4-(4-methoxyphenylpentyl), 138-9.5.degree.; (dl) Ph, 2-(4-fluorophenyl)propyl, 214.5-20.degree. (HCl); (dl) Ph, 2-(4-fluorophenyl)butyl, 174-81.degree.; (dl) Ph, 3-(4-fluorophenyl)butyl; 155-8.5.degree.; (dl) Ph, 4-(4-fluorophenyl)pentyl, 129.5-32.degree.; (dl) Ph, 4-(4-chlorophenyl)pentyl, 146-7.degree.; Ph, 4-(4-chlorophenyl)-3-pentenyl, 181-3.degree.; (dl) Ph, 2-phenyl-1-cyclopropylmethyl, 170-84.degree.; (dl) Ph, 3-methoxy-3-phenylpropyl, 162-4.degree.; Ph, 5-phenylpentyl, 143-4.5.degree.; Bu, 3-(4-fluorobenzoyl)propyl, 209-13.5.degree. (2HCl.H2O); Ph, 4-(4-fluorophenyl)-3-butenyl, 204-5.degree.; Ph, 4-(4-methylphenyl)-3-pentenyl, 170-4.5.degree.; Ph, 4-(4-methoxyphenyl)-3-pentenyl, 136-45.degree.; Ph, 4-phenyl-3-pentenyl, 216-18.degree. (HCl); Ph, 4-(4-fluorophenyl)-3-pentenyl, 163-4.5.degree.; Ph, 4,4-diphenylbutyl, 204-6.degree.; Ph, 5,5-diphenylpentyl, 195.5-96.degree.; (dl) Ph, 4-(4-methylphenyl)-4-phenylbutyl, 166-86.degree.; (dl) Ph, 4-(4-methoxyphenyl)-4-phenylbutyl, 176-8.degree.; (dl) Ph, 4-(4-fluorophenyl)-4-phenylbutyl, 170-2.degree.; (dl) Ph, 5-(4-fluorophenyl)-5-phenylpentyl, 182.5-3.5.degree.; (dl) Ph, 4-(4-fluorophenyl)-4-(4-methylphenyl)butyl, 161-3.5.degree.; Ph, 4,4-bis(4-fluorophenyl)butyl, 187.5-90.degree.; Ph, 5,5-bis(4-fluorophenyl)pentyl, 265-6 (HCl); (dl) Ph, 4-(4-fluorophenyl)-4-(3-trifluoromethylphenyl)butyl, 247-8.degree. (HCl); Ph, 4,4-bis(3-trifluoromethylphenyl)butyl, 246-9.degree. (HCl); (dl) Ph, 4-(4-fluorophenyl)-4-(2-thienyl)butyl, 202-3.degree.; (dl) Ph, 5-(4-fluorophenyl)4-phenylpentyl, 191-3.5.degree.; (dl) Ph, 4,5-bis(4-fluorophenyl)pentyl, 141-3.degree.; Ph, 5,5-diphenyl-4- pentenyl, 195.5-97; Ph, 4-(4-methylphenyl)-4-phenyl-3-butenyl, 174.5-88.degree.; Ph, 4-(4-methoxyphenyl)-4-phenyl-3-butenyl, 169-73.degree.; Ph, 4-(4-fluorophenyl)-4-phenyl-3-butenyl 180-4.degree.; Ph, 5-(4-fluorophenyl)-5-phenyl-4-pentenyl, 197-8.5.degree.; Ph, 4-phenyl-4-(3-trifluoromethylphenyl)-3-butenyl, 179.5-85.5.degree.; Ph, 4,4-bis(4-methylphenyl)-3-butenyl, 183-4.degree.; Ph, 4,4-bis(4-methoxyphenyl)-3-butenyl, 221-8.degree.; Ph, 4,-(4-fluorophenyl)-4-(4-methoxyphenyl)-3-butenyl, 242-4.degree. (HCl); Ph, 4,4-bis(4-fluorophenyl)-3-butenyl, 189.5-93.degree.; Ph, 4-(4-chlorophenyl)-4-(4-fluorophenyl)-3-butenyl, 252-3.degree. (HCl); Ph, 4,4-bis(3-trifluoromethyl)phenyl)-3-butenyl, 233-7.5.degree.; Ph, 5,5-bis(4-fluorophenyl)-4-pentenyl, 154-8.degree.; Ph, 4-(4-fluorophenyl)-4-(3-trifluoromethylphenyl)-3-butenyl, 226-9.degree. (HCl); Ph, 4-(4-fluorophenyl)-4-(4-methylphenyl)-3-butenyl, 163-6.degree.; Ph, 4-(4-fluorophenyl)-4-(2-thienyl)-3-butenyl, 236-44 .degree. (HCl); Ph, 5-(4-fluorophenyl)-4-phenyl-3-pentenyl, 147-57.degree.; Ph, 4,5-bis(4-fluorophenyl)-3-pentenyl, 162-4.degree.; Ph, 5-phenoxypentyl, 170-1.5.degree.; Ph, 3-(2-methylphenoxy)propyl, 188-9.degree.; Ph, 3-(3-methylphenoxy)propyl, 159-9.5.degree.; Ph, 3-(4-methylphenyl)propyl, 165-6.degree.; Ph, 3-(4-methoxyphenoxy)propyl, 164-5.5.degree.; Ph, 3-(3-methoxyphenoxy)propyl, 166-7.degree.; Ph. 3-(2-fluorophenoxy)propyl, 173.5-75.degree.; Ph, 2-(diphenylmethoxy)ethyl, 176-80.degree.; Ph, 3-(3-fluorophenoxy)propyl, 152-4.degree.; Ph,3-(4-fluorophenoxy)propyl, 173.2-4.4.degree.; HCl salt 207-12.degree.; Ph, 2-(phenylthio)ethyl, 178-80.degree.; Ph, 3-(phenylthio)propyl, 185.5-6.5.degree.; Ph, 3-(4-methylthiophenoxy)propyl, 163.5-4.5.degree.; Ph, 2-(4- fluorothiophenoxy)ethyl 146-50.degree., Ph, 3-(4-fluorophenylthio)propyl, 168.5-69.degree.; Ph, 2-[.alpha.-(4-fluorophenyl)benzyloxy]ethyl, 166-8.degree.; Ph, 2-[bis(4-fluorophenyl)methoxy]ethyl, 163-4.degree.; (dl) Pr, 5-(4-fluorophenyl)-5-hydroxy-5-phenylpentyl, 151-5.degree.; Ph, 5,5-bis(4-fluorophenyl)-5-hydroxypentyl, 126-83.degree. (decompn.) (oxalate); Ph, Pr, 201.5-203.degree.; Ph, 4-cyano-4,4-diphenylbutyl, 212-13.5.degree.; Ph, 5-cyano-5,5-

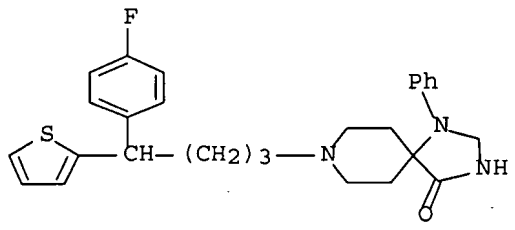
diphenylpentyl, 187.5-88.degree.; Ph, 2-benzyloxyethyl, 147-50.degree.; Ph, 3-methyl-2-butenyl, 180-2.degree.; Ph, 4-cyclopropyl-3-butenyl, 200-6.degree.; Ph, 2-hydroxyethyl, 180-5.5.degree.; Ph, 2-(benzoyloxy)ethyl, 191-3.degree.; (dl) Ph, 4-hydroxy-4-phenylbutyl, 154-61.degree.; (dl) Ph, 5-hydroxy-5-phenylpentyl, 174-4.5.degree.; (dl) Ph, 4-(4-fluorophenyl)-4- propionoxybutyl, 219-22.degree. (HCl); (dl) Ph, 4-(4-fluorophenyl)-4- acetoxybutyl, 158.5-60.degree.; (dl) Ph, 2-hydroxy-2-phenylethyl, 173-7.degree.; Ph, 4,4-diphenyl-3-butenyl, 201.5-207.degree.; Ph, 2-benzoylethyl, 159-63.degree.; (dl) Ph, 2-phenylpropyl, 144-52.degree.; (dl) Ph, 1-phenylethyl, 217-18.degree.; (dl) Ph, 2-(1,4- benzodioxanyl)methyl, 143-3.6.degree.; Bu, 3-cyano-3,3-diphenylpropyl, 246-54.degree. (2HCl); cyclohexyl, 4,4-diphenylbutyl, 207-10.degree.; Ph, 5,5-diphenyl-4-pentenyl, 195.5-97.degree.. The following V were also prepd. (R1, R2, R3, and m.p. given): Ph, Me, 3-(4-fluorobenzoyl)propyl, 252-4.degree.; Ph, Me, H, 205-9.degree. (HCl); (dl) Ph, Me, 4-(4-fluorophenyl)-4-phenylbutyl, 149-51.degree.; Ph, 2-cyanoethyl, H, 265-8.degree. (HCl); Ph, 2-cyanoethyl, 4,4-bis(4-fluorophenyl)butyl, 125-37.degree. (HCl); Ph, Me, 4,4-bis(4-fluorophenyl)butyl, 233-43.degree. (HCl). The following compds. were prepd. by conventional methods (b.p./mm., n20D, and d2020 given): dl-1-chloro-4-(4-methylphenyl)pentane, 94-5.degree./0.2,, 1.5102, 0.9918; dl-1-bromo-2(4-fluorophenyl)propane, 74-7.degree./0.9, -, -; dl-.alpha.-(ethoxycarbonyl)-4-fluorobenzyl cyanide, 112-13.degree./1, 1.4900, 1.1655; dl-2-(ethoxycarbonyl)-.alpha.- ethyl-4-fluorobenzyl cyanide, 107-10.degree./0.7, 1.4841, 1.1154; dl-2-(4-fluorophenyl)butyronitrile, 124-5.degree./15, 1.4903, 1.0578; dl-2-(4-fluorophenyl)butyric acid, 120-3.degree./1.1,-, -; dl-2-(4-fluorophenyl)butanol, 126-7.degree./17.5, 1.5003, 1.072; dl-1-bromo-2-(4-fluorophenyl)butane, 113-17.degree./12, -, -; dl-1-bromo-4-(4-fluorophenyl)pentane, 141-1.5.degree./16, -, -; dl-4-chlorophenyl(cyclopropyl)(methyl) carbinol, 102-4.degree./1, 1.5485, 1.1498; 5-chloro-2-(4-chlorophenyl)-2-pentene, 128-31.degree./1.5, 1.5696, 1.1694; dl-1-chloro-4-(4-chloropentyl)pentane, 115-17.degree./1.5, 1.5291, 1.1244; dl-1-(bromomethyl)-2-phenylcyclopropane, 72-87.degree./0.5, 1.5662, 1.3100; 4-chloro-1-(4-fluoro-phenyl)-1-butene, 130-2.degree./12, -, -; dl-cyclopropyl(methyl) (4-methylphenyl) carbinol, 110-15.degree./0.9-2, -, -; 5-chloro-2(4-methylphenyl)-2-pentene, 99-103.degree./0.9, 1.5500, 1.0407; dl-cyclopropyl(4- methoxyphenyl)(methyl)carbinol, 143.degree./3, 1.5432, 1.0720; 5-chloro-2-(4-methoxyphenyl)-2-pentene, 141-3.degree./2, 1.5578, 1.1080; 5-bromo-2-phenyl-2-pentene, 145-55.degree./19,-, -; 5-bromo-2-(4- fluorophenyl)-2-pentene, 133-6.degree./10, 1.5500, 1.3384; 1-chloro-4,4-diphenylbutene, 180-5.degree./2, 1.5728, 1.0874; 5-chloro-1,1-diphenylpentanol, - (m. 58-61.degree.), -, -; 5-chloro-1,1-diphenyl-1-pentene, 150-65.degree./1.5, -, -; 1-chloro-5,5-diphenylpentane, 130-44.degree./0.2, -, -; dl-cyclopropyl(4-methylphenyl)(phenyl) carbinol, 131-4.degree./0.4, 1.5795, -; 4-chloro-1 - (4 - methylphenyl) - 1 - phenyl- 1 -butene, 169-5.degree./1.4, 1.5955, -; dl-1-chloro-4-(4-methylphenyl)-4-phenylbutane, 140-2.degree./0.3, -, -; dl-cyclopropyl(4-methoxyphenyl)(phenyl)carbinol, 150-80.degree./1.5, 1.5890, 1.1417; 4-chloro-1-(4-methoxyphenyl)-1-phenyl-1-butene, 165-83.degree./0.4, -, -; dl-cyclopropyl-(4-fluorophenyl)phenyl) carbinol, 170-5.degree./6, -, -; 4-chloro-1(4-fluorophenyl)-1-phenyl-1-butene, 153-8.degree./1.2, -, -; dl-1 - chloro - 4 - (4 - fluorophenyl) - 4 - phenylbutane, 145-50.degree./0.2, 1.5578, 1.1447; dl-cyclopropyl(4- fluorophenyl)(4-methylphenyl)carbinol, 130-5.degree./0.4, -, -; 4-chloro-1-(4-fluorophenyl)-1-(4- methylphenyl)-1-butene, 164-7.degree./2, 1.5809, -; 5-chloro-1-(4-fluorophenyl)-1-phenyl-1-pentene, 150-60.degree./0.6, -, -; dl-1-chloro-5- (4-fluorophenyl)-5-phenylpentane, 155-7.degree./0.6, -, -; 4-chloro-1,1-bis(4-fluorophenyl)-1-butene, 165-7.degree./6, 1.5698, 1.2151; 1-chloro-4,4-bis(4-fluorophenyl)butane, 166-8.degree./6, 1.5425, 1.2039; 5-chloro-1,1-bis(4-fluorophenyl)pentanol, (m. 50-5.degree.), -, -; 5-chloro-1,1-bis(4-fluorophenyl)-1-pentene, 127-42.degree./0.2, 1.5590, -; 1-chloro-5,5-bis(4-fluorophenyl)pentane, 100-30.degree./0.2, -, -; dl-cyclopropyl(4-fluorophenyl)(3- trifluoromethylphenyl) carbinol, 145-50.degree./1.5-2.degree., -, -; dl-1-chloro-4-(4-fluorophenyl)-

4-(3-trifluoromethylphenyl)butane, 140-5.degree./0.6, 1.5132, 1.2642; cyclopropylbis(3-trifluoromethylphenyl) carbinol, 137-9.degree./1.5, -, -; 4-bromo-1,1-bis(3- trifluoromethylphenyl)-1-butene, 145-7.degree./0.8, -, -; 1-bromo-4,4-bis(3-trifluoromethylphenyl)butane, 144-6.degree./0.4, -, -; dl-cyclopropyl(4-fluorophenyl)(2-thienyl) carbinol, 138-40.degree./1, 1.5777, 1.2296; 4-(4-fluorophenyl)4-(2-thienyl)but-3-en-1-ol, oil, -, -; dl-4-(4-fluorophenyl)-4-(2-thienyl)butanol, 147-56.degree./0.2-0.3, -, -; dl-1-chloro-4-(4-fluorophenyl)-4-(2-thienyl)butane, 140-2.degree./0.4, 1.5647, -; dl-1-cyclopropyl-2-(4-fluorophenyl)-1-phenylethanol, 160-70.degree./0.8, -, -; 5-chloro-1-(4-fluorophenyl)-2-phenyl-2-pentene, 165-70.degree./0.4, -, -; dl-1-chloro-5-(4-fluorophenyl)-4-phenylpentane, 145-50.degree./0.8 -, -; dl-1-cyclopropyl-1,2-bis(4-fluorophenyl)ethanol, 120-8.degree./0.09, -, -; 5-chloro-1,2-bis(4-fluorophenyl)-2-pentene, 144-6.degree./0.6, -, -; dl-1-chloro-4,5-bis(4-fluorophenyl)pentane, 114-29.degree./0.1, -, -; dl-cyclopropyl(phenyl)(3-trifluoromethylphenyl) carbinol, 144-6.degree./2.5, -, -; 4-chloro-1-phenyl-1-(3-trifluoromethylphenyl)-1- butene, 138-9.degree./0.6, 1.5470, 1.2255; cyclopropylbis(4-methylphenyl) carbinol, 171-5.degree./1.5, -, -; 4-chloro-1,1-bis(4-methylphenyl)-1- butene, 162-4.degree./0.6, 1.5907, -; 4-chloro-1,1-bis(4-methoxyphenyl)-1- butene, 210-12.degree./1, -, -; dl-cyclopropyl(4-fluorophenyl)(4- methoxyphenyl) carbinol, 138-42.degree./0.2-0.3, 1.5697, -; 4-chloro-1-(4-fluorophenyl)-1-butene, 162-5.degree./0.4, -, -; dl-4-chlorophenyl(cyclopropyl)(4-fluorophenyl) carbinol, 148-55.degree./ 0.6, 1.5787, 1.2425; 4-chloro-1-(4-chlorophenyl)-1-(4-fluorophenyl)-1- butene, oil, 1.5903, 1.2361; dl-cyclopropyl(4-fluorophenyl)(2-thienyl) carbinol, 138-40.degree./1, 1.5777, 1.2296; 4-chloro-1-(4-fluorophenyl)-1- (2-thienyl)-1-butene, 150-60.degree./0.6, -, -; 1-chloro-3-(4- methylthiophenoxy)propane, 152-6.degree./10, -, -; 2-(4- fluorothiophenoxy)ethanol, 111-20.degree./1, -, -; 1-chloro-2(4- fluorothiophenoxy)ethane, 122-3.degree./14, 1.5560, 1.2613; dl-5-chloro-1-(4-fluocophenyl)-1-phenylpentanol, 170-5.degree./0.8, -, -. The title compds. are used as central nervous system depressants.

IT 1810-49-7P, 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[4-(p-fluorophenyl)-4-(2-thienyl)butyl]-1-phenyl-, (.+-.)- 92247-13-7P, 2-Thiophenebutanol, .delta.-(p-fluorophenyl)-, (.+-.)- 92252-89-6P, Thiophene, 2-[.alpha.-(3-chloropropyl)-p-fluorobenzyl]-, (.+-.)-
RL: PREP (Preparation)
(prepn. of)

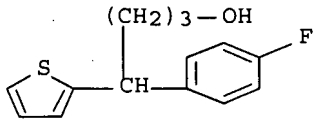
RN 1810-49-7 CAPLUS

CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[4-(p-fluorophenyl)-4-(2-thienyl)butyl]-1-phenyl- (7CI, 8CI) (CA INDEX NAME)

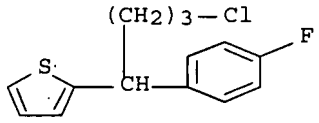


RN 92247-13-7 CAPLUS

CN 2-Thiophenebutanol, .delta.-(p-fluorophenyl)- (7CI) (CA INDEX NAME)



RN 92252-89-6 CAPLUS
CN Thiophene, 2-[.alpha.-(3-chloropropyl)-p-fluorobenzyl]- (7CI) (CA INDEX NAME)



L6 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:50526 CAPLUS Full-text
DOCUMENT NUMBER: 52:50526
ORIGINAL REFERENCE NO.: 52:9067f-i,9068a-h
TITLE: Decomposition reactions of heterocyclic diacyl peroxides. II. 2-Thenoyl peroxide
AUTHOR(S): Ford, M. C.; Mackay, Donald
CORPORATE SOURCE: Univ. Old Aberdeen, UK
SOURCE: Journal of the Chemical Society (1957) 4620-5
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

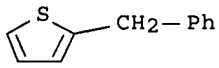
AB cf. C.A. 45, 9027h. Compds. formed by the decompn. of 2-thenoyl peroxide (I) in aromatic solvents can be attributed largely to reactions of 2-thenoyloxy radicals. The most regular feature was the formation of aryl 2-thenoates, in low yield, by nuclear attack, and in the halobenzenes phenyl 2-thenoate (II) was formed, with displacement of the halogen. In PhMe and cumene (III) attack occurred preferentially in the side chain. In solvents lacking side chain H, the formation of 2-thenoic anhydride (IV) was sometimes observed. In thiophene (V), 2-thienyl 2-thenoate (VI) and 2,2'-bi-thienyl (VII) were produced, VII providing evidence for the generation of 2-thienyl radicals. 2-Thenoic acid (VIII), m. 127-8.degree., with SOCl2 gave a nearly quant. yield of the acid chloride (IX), b10 77.degree.. The following esters of VIII were prepd. under Schotten-Baumann conditions from the appropriate phenol: II, m. 54.degree.; 1-naphthyl (X), m. 80.degree.; p-ClC6H4 (XI), m. 84-4.5.degree.; p-BrC6H4 (XII), m. 85.degree.; VI, m. 54.degree.; p-O2NC6H4, (XIII), m. 181.degree. (MeOH). IX (14 g.) in 20 ml. cyclohexane stirred 20 min. with 40 ml. 2N NaOH and 50 ml. 30-vol. H2O2 gave 60-5% I, prisms, m. 103.degree. (C6H6-ligroine). The decompns. of I in C6H6, the halobenzenes, and nitrobenzenes were carried out in the dark, and on an oil bath. Working up consisted in removal of the solvent in vacuo, extn. with Et2O, and sepn. of the acid by repeated shaking with 2N KHCO3. Except in the case of the PhMe decompn., the acid was obtained pure after recrystn. from H2O. After drying of the Et2O soln. the solvent was removed and the neutral residue treated as described. I (6.0 g.) decompd. in 600 ml. C6H6 48 hrs. at 75-85.degree. under N evolved 0.26 mole CO2; the solvent removed, and the resulting tar extd. with Et2O gave 1.9 g. VIII and neutral material which, distd. at 0.01 mm., yielded

0.7 g. of an oil, and chromatography on anhyd. MgSO4 gave 0.2 g. II, m. 53.degree. and 0.3 g. IV, m. 60.5-1.5.degree. (ligroine). In another expt. 750 mg. I decompd. during 24 hrs. in 75 ml. C6H6, the solvent removed through a short column, and the distillate tested with isatin in concd. H2SO4 showed that the mixt. contained 1 mg. V. I (1.0 g.) heated 10 hrs. at 80-90.degree. with 20 g. C10H8 in 20 ml. C6H6 gave 0.54 g. VIII and 0.1 g. X. Decompn. of 12 g. I in 1180 ml. PhNO2 36 hrs. at 85-95.degree. similarly gave 2.7 g. VIII and 50 mg. crude XIII. I (18 g.) heated 45 hrs. at 65-75.degree. in 1620 ml. PhCl and the neutral material distd. at 0.01 mm. chromatography on MgSO4 gave 1.4 g. material which, rechromatographed on Norit, yielded 0.38 g. II, 0.02 g. XI, and 0.17 g. VI. The 2nd fraction of 1.4 g. rechromatographed on MgSO4 from ligroine gave IV, m. 59.5.degree. (ligroine). In a similar expt., in which 9 g. I gave 0.24 g. II, the total combined Cl was found to amt. 0.11 g. I (15 g.) decompd. 24 hrs. at 75-80.degree. in 1400 ml. PhBr, distd., and chromatographed on Norit gave 0.17 g. II and 0.26 g. XII. I (7 g.) in 100 ml. PhBr added during 3 hrs. to 500 ml. PhBr under reflux with the effluent gases passed through acidified AgNO3 and refluxed a further hr. gave 2.1 millimoles AgBr and 2.6 g. VIII, 0.57 g. II, and a trace of XII. I (2.5 g.) in 60 ml. PhI added all at once to 190 ml. PhI at 150.degree., and the whole heated 5 min. at 150.degree. gave 0.9 g. VIII, 0.12 g. II, and 30 mg. IV. The liberated iodine was extd. with satd. aq. KI and titrated with 0.1N thiosulfate. I (18 g.) decompd. 48 hrs. at 75-85.degree. in 1700 ml. PhMe gave 12.5 g. acidic material shown to contain 11 g. pure VIII. Trituration of the insol. fraction gave 0.17 g. 5(?)-(2-thenoyloxy)-2-thenoic acid (XIV), prisms, m. 195.degree. (decompn.). XIV with CH2N2 gave the Me ester, m. 131-2.degree. (decompn.)(ligroine). XIV on hydrolysis gave VIII, together with a highly sol. hydroxythenoic acid, which with aq. FeCl3 formed an intense vermilion color, rapidly changing to a dark red ppt. The residue from the org. layer gave 4.5 g. material, b0.01 70-80.degree., which on recrystn. yielded Ph2, m. 48-50.degree., and the mother liquor evapd. and the residue chromatographed on Al2O3 gave 2.9 g. more Ph2 and 2-benzylthiophene (XV) characterized by conversion to 2-benzyl-5- (chloromercuri)thiophene, prisms, m. 184-5.degree. (MeOH-CHCl3). The 2nd fraction (1.5 g.) refluxed 0.5 hr. with 4 g. KOH in 25 ml. alc., the alc. removed, H2O added, and the soln. extd. with Et2O gave 0.4 g. PhCH2OH; phenylcarbamate, m. 76-7.degree.. The alk. soln. gave 0.7 g. VIII and 0.2 g. phenolic material, which with 1-C10H7NCS yielded .omicron.-tolyl .alpha.-naphthylcarbamate, m. 136.degree.. In another expt. (1 g. I in 95 ml. PhMe) the effluent N was passed through a trap at -70.degree. and the solvent distd., giving about 0.2 mg. V. I (3.0 g.) in 300 ml. III 36 hrs. at 70-80.degree. gave 3 g. VIII and 0.24 g. (Me2CPh)2, m. 117.degree. (MeOH). I (3.0 g.) in 100 ml. V refluxed 16 hrs. gave 1.3 g. VIII, and distn. of the org. fraction yielded 0.50 g. VI. The ligroine-sol. fraction chromatographed on MgSO4 yielded 0.12 g. VII, m. 34-5.degree., and 0.73 g. more VI. Bz2O2 (4.0 g.) in 100 ml. V refluxed 24 hrs. and similarly worked up gave 2.6 g. BzOH and 0.51 g. 2-thienyl benzoate, m. 43-4.degree.. I (3 g.) added in small portions to 6 g. Et2S and refluxed 3 min. after the exothermic reaction had occurred gave 1.9 g. VIII and 0.63 g. IV. Similarly 8 g. Bz2O2 with 16 g. Et2S gave 5 g. BzOH and 1.3 g. Bz2O. In neither case was any attempt made to isolate the oxidation products of the sulfide. (tert-BuO)2 (10 g.), 50 ml. PhMe, and 50 ml. V refluxed 7 days and concd. gave a high-boiling residue which, extd. with ligroine, yielded 0.5 g. XV. No (PhCH2)2 was formed.

IT 13132-15-5P, Thiophene, 2-benzyl-
RL: PREP (Preparation)
(prepn. of)

RN 13132-15-5 CAPLUS

CN Thiophene, 2-(phenylmethyl)- (CA INDEX NAME)



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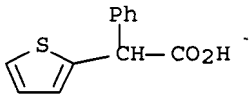
ACCESSION NUMBER: 1954:64543 CAPLUS
DOCUMENT NUMBER: 48:64543
ORIGINAL REFERENCE NO.: 48:11500e-i
TITLE: 1-Methylpiperidinemethanols
INVENTOR(S): Feldkamp, Rolland F.
PATENT ASSIGNEE(S): Sterling Drug Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2657211		19531027	US 1951-246339	19510912

AB 1-Methylpiperidinecarboxylates (I) are prepd. by catalytically hydrogenating a lower-alkyl pyridinecaxboxylate in a liquid inert to H (e.g., EtOH, dioxane, Et2O, methylcyclohexane, or 20-35% aq. HOAc), N-methylating and concurrently hydrogenating the resultant alkyl piperidinecarboxylate by adding excess aq. HCHO and a catalyst, followed by H under pressure, filtering, neutralizing with aq. KOH, extg. with Et2O, drying, and distg. Catalysts for the 1st hydrogenation are Pd, Pt, Ni, or Cu chromite; the first 3 also catalyze the 2nd hydrogenation. A I so prepd. is reduced to a 1-methylpiperidinemethanol (II) by heating with Na, PhMe, and an alkanol of 3-8 C atoms [e.g., Me2CHCH2CH(OH)Me] and sepg. the product. The method of Sandborn and Marvel (C.A. 22,963) leaves the ring unsatd. and hence their values for 1-methyl-3-piperidinemethanol (III) are in error. Likewise the values of Renshaw, et al. (C.A. 33, 3379), for III, for 1-methyl-2-piperidinemethanol (IV) and for derivs. of III and IV are wrong. More nearly correct values follow (V = 1-methyl-2-piperidinemethanol; VI = 1-methyl-3-piperidinemethanol): III, b17 113-15.degree., n25D 1.4761, d. 0.9649; VI diphenylacetate-HCl, m. 195-6.degree.; VI 4-nitrobenzoate-HCl, m. 232.8-34.5.degree.; III.MeI, m. 215.5-16.5.degree.; VI acetate-MeI, m. 130-1.degree.; V acetate-MeI, m. 145-6.degree.; IV.MeI, m. above 300.degree.. The m.ps. of other compds. are: V acetate-MeI, 145-6.degree.; VI acetate-MeI, 130-1.degree.; VI acetate-HCl, 167-8.5.degree.; VI benzoate-HCl, 177-8.degree.; VI benzoate-MeI, 196.5-7.0.degree.; VI nicotinate-2HCl.H2O, 147-9.degree.; VI 2-thenoate-HCl, 152-3.degree.; VI benzilate-HCl, 217.5-20.degree.; VI benzilate-MeBr, 227.5-30.degree.; VI phenyl(2-thienyl)acetate-HCl, 174.-5.5.degree.; VI 3-hydroxy-2-phenylbutanoate-MeI, 158-62.degree.; 1-methyl-4-piperidinemethanol acetate-MeI, 149.5-51.5.degree.. Esters of a II are prepd. by refluxing with an acid (preferably in the presence of HCl gas), acid halide, or acid anhydride. In the 1st-mentioned method (the best for esters of acids contg. thiophene or free OH groups), a H2O separator is used to shift the equil. favorably. Methiodides of the acetates of II are prepd. from II. MeI by refluxing 0.5 hr. with Ac2O. Cf. C.A. 45, 4271eg.

IT 6343-63-1, 2-Thiopheneacetic acid, .alpha.-phenyl-
(esters)
RN 6343-63-1 CAPLUS
CN 2-Thiopheneacetic acid, .alpha.-phenyl- (8CI) (CA INDEX NAME)



L6 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1940:4694 CAPLUS Full-text
DOCUMENT NUMBER: 34:4694
ORIGINAL REFERENCE NO.: 34:755e-i,756a-g
TITLE: Thiophene series. XLIX. Constitution of indophenins
AUTHOR(S): Steinkopf, Wilhelm; Hanske, Werner
SOURCE: Ann. (1939), 541, 238-60
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

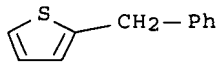
AB cf. C. A. 33, 8196.1. The Grignard reagent (I) from 53 g. of 2-iodothiophene (II) and 6 g. I in 100 cc. C6H6, added to 14.8 g. of isatin in 500 cc. C6H6 during 30 min., heated 15 min. and treated with 500 cc. 10% NaOH, gives 14.3 g. of 3-(2-thienyl)dioxindole (III), m. 208-8.5.degree.; heating with NaOH 0.5 hr. gives the Na salt of 2-thienyl-o-aminomandelic acid, the diazo compd. of which gives a red dye with .beta.-C10H7OH. III yields a di-Bz deriv., m. 159.degree.. Heating 3.5 g. of III with ZnCl2 at 180.degree. for 15 min. gives 40 mg. of isatin(thiophen)indophenin, which may be recrystd. from BzOEt or C5H5N; this is identical with the product prepd. by S. and Hempel (C. A. 26, 3793). I from 4.6 g. II and Et 5-bromoisatin-1-acetate in Et2O give 5.9 g. of Et 3-(2-thienyl)-5-bromodioxindole-1-acetate, m. 124-5.degree.; warming 3.7 g. in 150 cc. AcOH with 120 cc. concd. H2SO4 and 40 cc. AcOH at 55-60.degree. gives 0.15 g. of Et 5-bromoisatin (thiophen)-1-acetate, blue (S. and H.). The I from 5.3 g. of II in 20 cc. C6H6 and 3 g. of 1-methylisatin in 100 cc. C6H6 give 1.5 g. of 1-methyl-3-(2- thienyl)dioxindole, m. 127.5-9.degree., which gives the indophenin with AcOH-H2SO4. 5-Bromo-3-(2-thienyl)dioxindole, m. 217.5.degree. (decompn.); AcOH-H2SO4 gives the indophenin. The I from 10.6 g. of II and 8.8 g. of Et mesoxalate in Et2O give mesoxophenin (di-Et mesoxalate (thiophen)indophenin) (IV); hydrolysis with KOH in dioxane-MeOH gives the yellow-red K salt of glyoxylic acid(thiophen)indophenin. IV and Zn in AcOH give di-Et 2,2'-dithienyl-5,5'-bis(malonate), pale yellow, m. 111.5-12.5.degree.; hydrolysis with KOH in EtOH (30 min.) and acidification with 50% AcOH give 2,2'-dithienyl-5,5'-bisacetic acid, m. 217.degree.; Me ester, yellow, m. 75.5-7.degree.; decarboxylation gives 5,5'-dimethyl-2,2'-bithienyl (VI), m. 65.5-6.5.degree.. The I from 5.3 g. of II and PhCOCO2Et (VIA) give 2 g. of Et .alpha.-(2-thienyl)mandelate (VII), b0.3 136.degree., m. 59.5-60.5.degree.; 0.8 g. of the ester with 20 cc. concd. H2SO4, shaken for 5 min., gives 10 mg. of Et phenylglyoxylate(thiophen)indophenin (VIII), red-violet, m. 208.degree., which has a green metallic luster on rubbing; this also results on melting VII with ZnCl2 and in 0.9-g. yield from 4.2 g. of VIA and 3 g. thiophene in 320 cc. petr. ether at 0.degree. with 55 cc. ice-cold H2SO4; the free acid (IX) m. 208-10.degree. (decompn.); the K salt forms red needles. VIII with Zn in boiling AcOH gives the Et ester, pale yellow, m. 95-6.5.degree., of 2,2'-bithienyl-5,5'-bis(.alpha.-phenylacetic acid), yellow, m. 70-85.degree. (decompn.); decarboxylation gives VI. 2,2'-Bithienyl (3.4 g.) and 9 g. of BzCl in C6H6 with 7 g. TiCl4 give 1.2 g. 5,5'-dibenzoyl-2,2'-bithienyl (X), orange, m. 250-2.degree.; this also results from IX in NH3; concd. H2SO4 gives an intense green-yellow fluorescence; Zn in AcOH gives a blue-red color. X yields a 3,3'-di-Br deriv., pale reddish yellow, m. 195-7.degree.. The I from 10.5 g. II and 10.5 g. of benzil give a yellow-white ppt. which with CH2N2 yields the Me ether of ms-(2-thienyl)desoxybenzoin (XI), m. 71-2.degree.. XI

(80 g.) in 500 cc. AcOH and 500 cc. concd. H2SO4 in 900 cc. AcOH at 45-50.degree. for 20 min. give benzil(thiophen)indophenin (XII), golden green, becoming blue on rubbing, m. 223.degree.. Benzil and thiophene in CHCl3, shaken with concd. H2SO4 give ms-bis(2-thienyl)desoxybenzoin, m. 103.5-4.degree.. XII and Zn in AcOH give 5,5'-bis(phenylbenzoylmethyl)- 2,2'-bithienyl, m. 219.5-20.5.degree., which with EtONa gives 5,5'-dibenzoyl-2,2'-bithienyl (XIII), m. 96.5-7.5.degree.. This proves the presence of a 2,2'-bithienyl nucleus in indophenins. Thiophene (30 g.) and 30 g. PhCH2OH with 30 g. ZnCl2, gently boiled 0.5 hr., give (from 100 g. thiophene in 3 lots) 42 g. of recovered thiophene, 51 g. of 2-benzylthiophene, b1 257-62.degree., and 23 g. of 2,5-dibenzylthiophene, b12 220-2.degree.. 5-Chloromercuri-2-benzylthiophene with I-KI at 50.degree. gives 5-iodo-2-benzylthiophene, m. 55-7.degree.; with Naturkupfer C at 185-90.degree. and then at 190-210.degree. there results 14% of XIII. I and Ac2 in Et2O give ms-(2-thienyl)acetone, pale yellow, b1 82.degree.. Cumaran-2,3-dione (15 g.) and 8.4 g. thiophene with concd. H2SO4 in AcOH (0.5 hr. at 55.degree.) give 90 mg. of cumaran-2,3-dione(thiophen)indophenin, green-gold, does not m. 300.degree.. The Grignard reagent from 9.8 g. of 5-iodo-2-thiotolene and 9.2 g. of benzil give 5.7 g. of ms-(2-methyl-5-thienyl)benzoin, m. 78-9.degree.; AcOH-H2SO4 gives a blue color, which, quickly turns to a dirty red-brown; heating with BzOH at 180.degree. gives a blue powder. The Grignard reagent from 2,5-dibromothiophene gives ms-(2-bromo-5-thienyl)benzoin, m. 99-100.5.degree.; cold concd. H2SO4 gives only a yellow halochromy; on warming the yellow color changes to blue but H2O ppts. only brown flakes. The action of CO2 upon the Grignard reagent from 2,5-diiodo-3-thiotolene gives 2-iodo-3-thiotolene-5-carboxylic acid, m. 172-3.degree.. Structures proposed for indophenins are discussed in the light of the above expts.

IT 13132-15-5P, Thiophene, 2-benzyl-
RL: PREP (Preparation)
(prepn. of)

RN 13132-15-5 CAPLUS

CN Thiophene, 2-(phenylmethyl)- (CA INDEX NAME)



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